Cognitive Constructivism and the Epistemic Significance of Sharp Statistical Hypotheses in Natural Sciences

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À Marisa e a nossos filhos,
Rafael, Ana Carolina, e Deborah.

"Remanso de rio largo, viola da solidão:
Quando vou p'ra dar batalha, convido meu coração."
Gentle backwater of wide river, fiddle to solitude:
When going to do battle, I invite my heart.

João Guimarães Rosa (1908-1967).
Grande Sertão, Veredas.

"Sertão é onde o homem tem de ter a dura nuca e a mão quadrada.
(Onde quem manda é forte, com astucia e com cilada.)
Mas onde é bobice a qualquer resposta,
é aí que a pergunta se pergunta."
"A gente vive repetido, o repetido...
Digo: o real não está na saída nem na chegada:
ele se dispõem para a gente é no meio da travessia."

Sertao is where a man's might must prevail,
where he has to be strong, smart and wise.
But where every answer is wrong,
there is where the question asks itself.
We live repeating the reapeated...
I say: the real is neither at the departure nor at the arrival:
It presents itself to us at the middle of the journey.

Contents

Preface

"Life is like riding a bicycle.
To keep your balance you must keep moving."
Albert Einstein.

The main goals of this book are to develop an epistemological framework based on Cognitive Constructivism, and to provide a general introduction to the Full Bayesian Significance Test (FBST). The FBST was first presented in Pereira and Stern (1999) as a coherent Bayesian method for accessing the statistical significance of sharp or precise statistical hypotheses. A review of the FBST is given in the appendices, including:

 a) Some examples of its practical application;
 b) The basic computational techniques used in its implementation;
 c) Its statistical properties;
 d) Its logical or formal algebraic properties;

The items above have already been explored in previous presentations and courses given. In this book we shall focus on presenting

 e) A coherent epistemological framework for precise statistical hypotheses.

The FBST grew out of the necessity of testing sharp statistical hypothesis in several instances of the consulting practice of its authors. By the end of the year 2003, various interesting applications of this new formalism had been published by members of the Bayesian research group at IME-USP, some of which outperformed previously published solutions based on alternative methodologies, see for example Stern and Zacks (2002). In some applications, the FBST offered simple, elegant and complete solutions whereas alternative methodologies offered only partial solutions and / or required convoluted problem manipulations, see for example Lauretto et al. (2003).

The FBST measures the significance of a sharp hypothesis in a way that differs completely from that of Bayes Factors, the method of choice of orthodox Bayesian statistics. These methodological differences fired interesting debates that motivated us to investigate more thoroughly the logical and algebraic properties of the new formalism. These investigations also gave us the opportunity to interact with people in communities that were interested in more general belief calculi, mostly from the areas of Logic and Artificial

Intelligence, see for example Stern (2003, 2004) and Borges and Stern (2007).

However, as both Orthodox Bayesian Statistics and Frequentist Statistics have their own well established epistemological frameworks, namely, Decision Theory and Popperian Falsificationism, respectively, there was still one major gap to be filled: the establishment of an epistemological framework for the FBST formalism. Despite the fact that the daily practice of Statistics rarely leads to epistemological questions, the distinct formal properties of the FBST repeatedly brought forward such considerations. Consequently, defining an epistemological framework fully compatible with the FBST became an unavoidable task, as part of our effort to answer the many interesting questions posed by our colleagues.

Besides compatibility with the FBST logical properties, this new epistemological framework was also required to fully support sharp (precise or lower dimensional) statistical hypothesis. In fact, contrasting with the decision theoretic epistemology of the orthodox Bayesian school, which is usually hostile or at least unsympathetic to this kind of hypothesis, this new epistemological framework actualy puts, as we will see in the following chapters, sharp hypothesis at the center stage of the philosophy of science.

Cognitive Constructivism

The epistemological framework chosen to the aforementioned task was Cognitive Constructivism, as presented in chapters 1 to 4, and constitute the core lectures of this course. The central epistemological concept supporting the notion of a sharp statistical hypothesis is that of a systemic eigen-solution. According to Heinz von Foerster, the four essential attributes of such eigen-solutions are: discreteness (sharpness), stability, separability (decoupling) and composability. Systemic eigen-solutions correspond to the "objects" of knowledge, which may, in turn, be represented by sharp hypotheses in appropriate statistical models. These are the main topics discussed of chapter 1.

Within the FBST setup, the *e-value* of a hypothesis, H, defines the measure of its *Epistemic Value* or the *Value of the Evidence* in support of H, provided by the observations. This measure corresponds, in turn, to the "reality" of the object described by the statistical hypothesis. The FBST formalism is reviewed in Appendix A.

In chapter 2 we delve into this epistemological framework from a broader perspective, linking it to the philosophical schools of Objective Idealism and Pragmatism. The general approach of this chapter can be summarized by the "wire walking" metaphor, according to which one strives to keep in balance at a center of equilibrium, to avoid the dangers of extreme positions that are faraway from it, see Figure J.1. In this context, such extreme positions are related to the epistemological positions of Dogmatic Realism and Solipsistic Subjectivism.

Chapters 3 and 4 relate to another allegory, namely, the Bicycle Metaphor: In a bike, it is very hard to achieve a static equilibrium, that is, to keep one's balance by standing still. Fortunately, it is easy to achieve a dynamic equilibrium, that is, to ride the bike running forward. In order to keep the bike running, one has to push the left and right pedals alternately, which will inevitably result in a gentile oscillation. Hence a double (first and second order) paradox: In order to stay in equilibrium one has to move forward, and in order to move forward one has to push left and right of the center. Overcoming the fear generated by this double paradox is a big part of learning to ride a bike.

Chapters 3 and 4 illustrate realistic and idealistic metaphorical pushes in the basic cycle of the constructivist epistemic ride. They work like atrial and ventricular systoles of a hart in the life of the scientific system. From an individual point of view, these realistic and idealistic pushes also correspond to an impersonal, extrospective or objective perspective versus a personal, introspective or subjective perspective in science making.

Chapter 5 explores the stochastic evolution of complex systems and is somewhat independent of chapters 1 to 4. In this chapter, the evolution of scientific theories is analyzed within the basic epistemological framework built in chapters 1 to 4. Also, while in chapters 1 to 4 many of the examples used to illustrate the topics under discussion come from statistical modeling, in chapter 5, many of the examples come from stochastic optimization.

Chapter 6 how some misperceptions in science or misleading interpretations can lead to ill-posed problems, paradoxical situations and even misconceived philosophical dilemmas. It also (re)presents some of the key concepts of Cog-Con using simple and intuitive examples. Hence, this last chapter may actually be the first one to read.

Figures J.2, J.3 and J.4 illustrate the bicycle metaphor. The first is a cartoon, by K.Przibram, of Ludwig Boltzmann, the second a photography of Albert Einstein, and the third a photography of Niels Bohr. They are all riding their bikes, an activity that appears to be highly beneficial to theoretical Probability. Boltzmann advocated for an atomistic and probabilistic interpretation of thermodynamics, that is, viewing thermodynamics as a limit approximation of Statistical Mechanics. His position was thoroughly rejected by the scientific establishment of his time. One of the main criticisms to his work was the introduction of "metaphysical", that is, non "empirical" or non "directly observable" entities. In 1905, annus mirabilis, Einstein published his paper on Brownian motion, providing a rigorous mathematical description of observable macroscopic fluctuation phenomena that could only be explained in the context of Statistical Mechanics. Sadly, Boltzmann died the next year, before his theories were fully appreciated. Discretization and probability are also basic concepts in Quantum Mechanics. The famous philosophical debates between Bohr and Einstein, involving these two concepts among others, greatly contributed to the understanding of the new theory.

Basic Tools for the (Home) Works

The fact that focus of this summer course will be on epistemological questions should not be taken as an excuse for working not so hardly with statistical modeling, data analysis, computer implementation, and the like. After all, this course will give to successful students 4 full credits in the IME-USP graduate programs!

In the core lectures we will illustrate the topics under discussion with several 'concrete' mathematical and statistical models. We have made a conscious effort to choose illustration models ivolving only mathematical concepts already familiar to our prospective students. Actually, most of these models are entail mathematical techniques that are used in the analysis and the computational implementation of the FBST, or that are closely related to them. Appendices A through K should help the students with their homeworks. We point out, however, that the presentation quality of these appendices is very heterogeneous. Some are (I hope) didactic and well prepared, some are only snapshots from slide presentations, and finally, some are just commented computer codes.

Acknowledgements and Final Remarks

The main goal of this book is to explore the FBST formalism and Bayesian statistics from a constructivist epistemological perspective. In order to accomplish this, ideas from many great masters, including philosophers like Peirce, Maturana, von Foerster, and Luhmann, statisticians like Peirce, Fisher, de Finetti, Savage, Good, Kemthorne, Jaynes, Jeffreys and Basu, ans physicists like Boltzmann, Planck, de Broglie, Bohr, Heisenberg, and Born have been used. I hope it is clear from the text how much I admire and feel I owe to these giants, even when my attitude is less then reverential. By that I mean that I always felt free to borough from the many ideas I like, and was also unashamed to reject the few I do not. The progress of science has always relied on the free and open discussion of ideas, in contrast to rigid cults of personality. I only hope to receive from the reader the same treatment and that, among the ideas presented in this work, he or she finds some that will be considered interesting and worthy of be kept in mind.

Chapters 1 to 4, released as Stern (2005a) and the Technical Reports Stern (2006a-c), have been used in January-February of 2007 (and again for 2008) in the IME-USP Summer Program for the discipline MAE-5747 Comparative Statistical Inference. Chapter 5, released as the Technical Report by Stern (2007c), has also been used in the second semester of 2007 in the discipline MAP-427 - Nonlinear Programming. A short "no-math" article based on part of the material in Chapter 1 has been published (in Portuguese) in the journal *Scientiae Studia*. Revised and corrected versions of articles based on the material presented at Chapters 1, 2 and 3 have also been either published or accepted for publication in the journal *Cybernetics & Human Knowing*. In the main text and the

appendices I have used several results concerning the FBST formalism, some of its applications, and also other statistical and optimization models and techniques, developed in collaboration with or by other researchers. Appropriate acknowledgements and references are given in the text.

The author has benefited from the support of FAPESP, CNPq, BIOINFO, the Institute of Mathematics and Statistics of the University of São Paulo, Brazil, and the Mathematical Sciences Department at SUNY-Binghamton, USA. The author is grateful to many people for helpful discussions, most specially, Wagner Borges, Soren Brier, Carlos Humes, Joseph Kadane, Luis Gustavo Esteves, Marcelo Lauretto, Fabio Nakano, Osvaldo Pessoa, Rafael Bassi Stern, Sergio Wechsler, and Shelemyahu Zacks. The author also received interesting comments and suggestions from the participants of FIS-2005, the Third Conference on the Foundations of Information Science, and several anonymous referees. The alchemical transmutation of my original drafts into proper English text is a non-trivial operation, in which I had the help of Wagner Borges and several referees.

But first and foremost I want to thank Professor Carlos Alberto de Bragança Pereira (Carlinhos). I use to say that he teached me much of the (Bayesian) Statistics I know, the easy part, after un-teaching me much of the (frequentist) Statistics I thought I knew, the hard part. Carlinhos is a lover of the scientific debate, based on the critical examination of concepts and ideas, always poking and probing established habits and frozen ideas with challenging questions. This is an attitude, we are told, he shared with his Ph.D. advisor, the late Prof. Debabrata Basu.

Just as an example, one of Carlinhos favorit questions is: Why do we (ever) randomize? I hope that some of the ideas presented in chapter 3 can contribute to the discussion of this fundamental issue. Carlinhos extensive consulting practice for the medical community makes him (some times, painfully) aware of the need of tempering randomization procedures with sophisticated protocols that take into account the patients' need of receiving proper care.

This work has its focus on epistemological aspects. The topics under discussion are, however, surprisingly close to, and have many times been directly motivated by, our consulting practice in statistical modeling and operations research. The very definition of the FBST was originally inspired by some juridical consulting projects, see Stern (2003). This does not mean that many of these interrelated issues tend to be ignored in everyday practice, like the proverbial bird that ignores the air which supports it, or the fish that ignores the water in which it swims.

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São Paulo, 20/12/2007.

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Version Control

- Version 1.0 - December 20, 2007.

- Version 1.1 - April 9, 2008. Several minor corrections to the main text and some bibliographic updates. The appendices have been reorganized as follows: Appendix A presents a short review of the FBST, including its definition and main statistical and logical properties; Appendix B fully reviews the distribution theory used to build Multinomial-Dirichlet statistical models; Appendix C summarizes several statistical models used to illustrate the core lectures; Appendix D (previously a separate handout) gives a short introduction to deterministic optimization; Appendix E reviews some important concepts related to the Maximum Entropy formalism and asymptotic convergence; Appendix F, on sparse factorizations, provides some technical details related to the discussions on decoupling procedures in chapter 3; Appendix G presents a technical miscellanea on Monte Carlo Methods; Appendix H provides a short derivation of some stochastic optimization algorithms and evolution models; Appendix I lists some open research programs; Appendix J contains all bitmap figures and, finally, Appendix K brings to bear pieces of difficult to get reading material. They will be posted at my web page, subject to the censorship of our network administrator and his understanding of Brazilian copyright laws and regulations. All computer code was removed from text and is now available at my web page, `www.ime.usp.br/∼jstern` .

This version has been used for a tutorial at MaxEnt-2008, the 28th International Workshop on Bayesian Inference and Maximum Entropy Methods in Science and Engineering, held on July 6-11, at Boracéia, São Paulo, Brazil.

- Version 1.2 - December 10, 2008. Minor corrections to the main text and appendices, and some bibliographic updates. New section F.1 on dense matrix factorizations. This section also defines the matrix notation now used consistently throughout the book.

- Version 2.0 - December 19, 2009. New section 4.5 and chapter 6, presented at the conference MBR'09 - Model Based Reasoning in Science and Technology - held at Campinas, Brazil. Most of the figures at exhibition in the art gallery are now in the separate file, `www.ime.usp.br/~jstern/pub/gallery2.pdf` .

Chapter 1

Eigen-Solutions and Sharp Statistical Hypotheses

"Eigenvalues have been found ontologically to be
discrete, stable, separable and composable ..."
Heinz von Foerster (1911 - 2002),
Objects: Tokens for Eigen-Behaviours.

1.1   Introduction

In this chapter, a few epistemological, ontological and sociological questions concerning the statistical significance of sharp hypotheses in the scientific context are investigated within the framework provided by Cognitive Constructivism, or the Constructivist Theory (ConsTh) as presented in Maturana and Varela (1980), Foerster (2003) and Luhmann (1989, 1990, 1995). Several conclusions of the study, however, remain valid, mutatis mutandis, within various other organizations and systems, see for example Bakken and Hernes (2002), Christis (2001), Mingers (2000) and Rasch (1998).

The author's interest in this research topic emerged from his involvement in the development of the Full Bayesian Significance Test (FBST), a novel Bayesian solution to the statistical problem of measuring the support of sharp hypotheses, first presented in Pereira and Stern (1999). The problem of measuring the support of sharp hypotheses poses several conceptual and methodological difficulties for traditional statistical analysis under both the frequentist (classical) and the orthodox Bayesian approaches. The solution provided by the FBST has significant advantages over traditional alternatives, in terms of its statistical and logical properties. Since these properties have already been thoroughly analyzed in previous papers, see references, the focus herein is directed exclusively to epistemological and ontological questions.

Despite the fact that the FBST is fully compatible with Decision Theory (DecTh), as shown in Madruga et al. (2001), which, in turn, provides a strong and coherent epistemological framework to orthodox Bayesian Statistics, its logical properties open the possibility of using and benefiting from alternative epistemological settings. In this chapter, the epistemological framework of ConsTh is counterposed to that of DecTh. The contrast, however, is limited in scope by our interest in statistics and is carried out in a rather exploratory an non exhaustive form. The epistemological framework of ConsTh is also counterposed to that of Falsificationism, the epistemological framework within which classical frequentist statistical test of hypotheses are often presented, as shown in Boyd (1991) and Popper (1959, 1963).

In section 2, the fundamental notions of Autopoiesis and Eigen-Solutions in autopoietic systems are reviewed. In section 3, the same is done with the notions of Social Systems and Functional Differentiation and in section 4, a ConsTh view of science is presented. In section 5, the material presented in sections 2, 3 and 4 is related to the statistical significance of sharp scientific hypotheses and the findings therein are counterposed to traditional interpretations such as those of DecTh. In section 6, a few sociological analyses for differentiation phenomena are reviewed. In sections 7 and 8, the final conclusions are established.

In sections 2, 3, 4, and 6, well established concepts of the ConsTh are presented. However, in order to overcome an unfortunately common scenario, an attempt is made to make them accessible to a scientist or statistician who is somewhat familiar with traditional frequentist, and decision-theoretic statistical interpretations, but unfamiliar with the constructivist approach to epistemology. Rephrasing these concepts (once again) is also avoided. Instead, quoting the primary sources is preferred whenever it can be clearly (in our context) and synthetically done. The contributions in sections 5, 7 and 8, relate mostly to the analysis of the role of quantitative methods specifically designed to measure the statistical support of sharp hypotheses. A short review of the FBST is presented in Appendix A.

1.2   Autopoiesis and Eigen-Solutions

The concept of autopoiesis tries to capture an essential characteristic of living organisms (auto=self, poiesis=production). Its purpose and definition are stated in Maturana and Varela (1980, p.84 and 78-79):

> *"Our aim was to propose the characterization of living systems that explains the generation of all the phenomena proper to them. We have done this by pointing at Autopoiesis in the physical space as a necessary and sufficient condition for a system to be a living one."*

> *"An autopoietic system is organized (defined as a unity) as a network of processes of production (transformation and destruction) of components that produces the components which:*
>
> *(i) through their interactions and transformations continuously regenerate and realize the network of processes (relations) that produced them; and*
>
> *(ii) constitute it (the machine) as a concrete unity in the space in which they (the components) exist by specifying the topological domain of its realization as such a network."*

Autopietic systems are non-equilibrium (dissipative) dynamical systems exhibiting (meta) stable structures, whose organization remains invariant over (long periods of) time, despite the frequent substitution of their components. Moreover, these components are produced by the same structures they regenerate. For example, the macromolecular population of a single cell can be renewed thousands of times during its lifetime, see Bertalanffy (1969). The investigation of these regeneration processes in the autopoietic system production network leads to the definition of cognitive domain, Maturana and Varela (1980, p.10):

> *"The circularity of their organization continuously brings them back to the same internal state (same with respect to the cyclic process). Each internal state requires that certain conditions (interactions with the environment) be satisfied in order to proceed to the next state. Thus the circular organization implies the prediction that an interaction that took place once will take place again. If this does not happen the system maintains its integrity (identity with respect to the observer) and enters into a new prediction. In a continuously changing environment these predictions can only be successful if the environment does no change in that which is predicted. Accordingly, the predictions implied in the organization of the living system are not predictions of particular events, but of classes of inter-actions. Every interaction is a particular interaction, but every prediction is a prediction of a class of interactions that is defined by those features of its elements that will allow the living system to retain its circular organization after the interaction, and thus, to interact again. This makes living systems inferential systems, and their domain of interactions a cognitive domain."*

The characteristics of this circular (cyclic or recursive) regenerative processes and their eigen (auto, equilibrium, fixed, homeostatic, invariant, recurrent, recursive) -states, both in concrete and abstract autopoietic systems, are further investigated in Foerster (2003) and Segal (2001):

> *"The meaning of recursion is to run through one's own path again. One of its results is that under certain conditions there exist indeed solutions which, when reentered into the formalism, produce again the same solution. These are called "eigen-values", "eigen-functions", "eigen-behaviors", etc., depending on which domain this formation is applied - in the domain of numbers, in functions, in behaviors, etc."* Segal (2001, p.145).

The concept of eigen-solution for an autopoietic system is the key to distinguish specific objects in a cognitive domain. von Foerster also establishes four essential attributes of eigen-solutions that will support the analyses conducted in this chapter and conclusions established herein.

> *"Objects are tokens for eigen-behaviors. Tokens stand for something else. In exchange for money (a token itself for gold held by one's government, but unfortunately no longer redeemable), tokens are used to gain admittance to the subway or to play pinball machines. In the cognitive realm, objects are the token names we give to our eigen-behavior.*
>
> *This is the constructivist's insight into what takes place when we talk about our experience with objects."* Segal (2001, p.127).
>
> *"Eigenvalues have been found ontologically to be discrete, stable, separable and composable, while ontogenetically to arise as equilibria that determine themselves through circular processes. Ontologically, Eigenvalues and objects, and likewise, ontogenetically, stable behavior and the manifestation of a subject's "grasp" of an object cannot be distinguished."* Foerster (2003, p.266).

The arguments used in this study rely heavily on two qualitative properties of eigen-solutions, refered by von Foerster by the terms "Discrete" and "Equilibria". In what follows, the meaning of these qualifiers, as they are understood by von Foerster and used herein, are examined:

a- Discrete (or sharp):

> *"There is an additional point I want to make, an important point. Out of an infinite continuum of possibilities, recursive operations carve out a precise set of discrete solutions. Eigen-behavior generates discrete, identifiable entities. Producing discreteness out of infinite variety has incredibly important consequences. It permits us to begin naming things. Language is the possibility of carving out of an infinite number of possible experiences those experiences which allow stable interactions of your-self with yourself."* Segal (2001, p.128).

It is important to realize that, in the sequel, the term "discrete", used by von Foerster to qualify eigen-solutions in general, should be replaced, depending on the specific context, by terms such as lower-dimensional, precise, sharp, singular etc. Even in the familiar case of linear algebra, if we define the eigen-vectors corresponding to a singular eigen-value c of a linear transformation $T(\ )$ only by its essential property of directional invariance, $T(x) = cx$, we obtain one dimensional sub-manifolds which, in this case, are subspaces or lines trough the origin. Only if we add the usual (but non essential) normalization condition, $||x|| = 1$, do we get discrete eigen-vectors.

b- Equilibria (or stable):

A stable eigen-solution of the operator $Op(\ )$, defined by the fixed-point or invariance equation, $x_{inv} = Op(x_{inv})$, can be found, built or computed as the limit, x_∞, of the sequence $\{x_n\}$, defined by recursive application of the operator, $x_{n+1} = Op(x_n)$. Under appropriate conditions, such as within a domain of attraction, the process convergence and its limit eigen-solution will not depend on the starting point, x_0. In the linear algebra example, using almost any staring point, the sequence generated by the recursive relation $x_{n+1} = T(x_n)/||T(x_n)||$, i.e. the application of T followed by normalization, converges to the unitary eigen-vector corresponding to the largest eigen-value.

In sections 4 and 5 it is shown, for statistical analysis in a scientific context, how the property of sharpness indicates that many, and perhaps some of the most relevant, scientific hypotheses are sharp, and how the property of stability, indicates that considering these hypotheses is natural and reasonable. The statistical consequences of these findings will be discussed in sections 7 and 8. Before that, however, a few other ConsTh concepts must be introduced in sections 3 and 6.

Autopoiesis found its name in the work of Maturana and Varela (1980), together with a simple, powerful and elegant formulation using the modern language of system's theory. Nevertheless, some of the basic theoretical concepts, such as those of self-organization and autonomy of living organisms, have long historical grounds that some authors trace back to Kant. As seen in Kant (1790, sec. 65) for example, a (self-organized) *"Organism"* is characterized as an entity in which,

> *"... every part is thought as 'owing' its presence to the 'agency' of all the remaining parts, and also as existing 'for the sake of the others' and of the whole, that is as an instrument, or organ."*

> *"Its parts must in their collective unity reciprocally produce one another alike as to form and combination, and thus by their own causality produce a whole, the conception of which, conversely, -in a being possessing the causality according to conceptions that is adequate for such a product- could in turn be the cause of the whole according to a principle, so that, consequently, the nexus of 'efficient causes' (progressive causation, nexus effectivus) might be no less*

estimated as an 'operation brought about by final causes' (regressive causation, nexus finalis)."

For further historical comments we refer the reader to Zelleny (1980).

1.3   Functional Differentiation

In order to give appropriate answers to environmental complexities, autopoietic systems can be hierarchically organized as Higher Order Autopoietic Systems. As in Maturana and Varela (1980, p.107,109), this notion is defined via the concept of Coupling:

> *"Whenever the conduct of two or more units is such that there is a domain in which the conduct of each one is a function of the conduct of the others, it is said that they are coupled in that domain."*

> *"An autopoietic system whose autopoiesis entails the autopoiesis of the coupled autopoietic units which realize it, is an autopoietic system of higher order."*

A typical example of a hierarchical system is a Beehive, a third order autopoietic system, formed by the coupling of individual Bees, the second order systems, which, in turn, are formed by the coupling of individual Cells, the first order systems.

The philosopher and sociologist Niklas Luhmann applied this notion to the study of modern human societies and its systems. Luhmann's basic abstraction is to look at social systems only at its higher hierarchical level, in which it is seen as an autopoietic communications network. In Luhmann's terminology, a communication event consists of: Utterance, the form of transmission; Information, the specific content; and Understanding, the relation to future events in the network, such as the activation or suppression of future communications.

> *"Social systems use communication as their particular mode of autopoietic (re)production. Their elements are communications that are recursively produced and reproduced by a network of communications that are not living units, they are not conscious units, they are not actions. Their unity requires a synthesis of three selections, namely information, utterance and understanding (including misunderstanding)."* Luhmann (1990b, p.3).

For Luhmann, society's best strategy to deal with increasing complexity is the same as one observes in most biological organisms, namely, differentiation. Biological organisms differentiate in specialized systems, such as organs and tissues of a pluricellular life form (non-autopoietic or allopoietic systems), or specialized individuals in an insect colony

(autopoietic system). In fact, societies and organisms can be characterized by the way in which they differentiate into systems. For Luhmann, modern societies are characterized by a vertical differentiation into autopoietic functional systems, where each system is characterized by its code, program and (generalized) media. The code gives a bipolar reference to the system, of what is positive, accepted, favored or valid, versus what is negative, rejected, disfavored or invalid. The program gives a specific context where the code is applied, and the media is the space in which the system operates.

Standard examples of social systems are:

- Science: with a true/false code, working in a program set by a scientific theory, and having articles in journals and proceedings as its media;

- Judicial: with a legal/illegal code, working in a program set by existing laws and regulations, and having certified legal documents as its media;

- Religion: with a good/evil code, working in a program set by sacred and hermeneutic texts, and having study, prayer and good deeds as its media;

- Economy: with a property/lack thereof code, working in a program set by economic planning scenarios and pricing methods, and having money and money-like financial assets as its media.

Before ending this section, a notion related to the break-down of autopoiesis is introduced: Dedifferentiation (Entdifferenzierung) is the degradation of the system's internal coherence, through adulteration, disruption, or dissolution of its own autopoietic relations. One form of dedifferentiation (in either biological or social systems) is the system's penetration by external agents who try to use system's resources in a way that is not compatible with the system's autonomy. In Lumann's conception of modern society each system may be aware of events in other systems, that is, be cognitively open, but is required to maintain its differentiation, that is, be operationally closed. In Luhmann's (1989, p.109) words:

"With functional differentiation... Extreme elasticity is purchased at the cost of the peculiar rigidity of its contextual conditions. Every binary code claims universal validity, but only for its own perspective. Everything, for example, can be either true of false, but only true or false according to the specific theoretical programs of the scientific system. Above all, this means that no function system can step in for any other. None can replace or even relieve any other. Politics can not be substituted for economy, nor economy for science, nor science for law or religion, nor religion for politics, etc., in any conceivable intersystem relations."

1.4   Eigensolutions and Scientific Hypotheses

The interpretation of scientific knowledge as an eigensolution of a research process is part of a constructive approach to epistemology. Figure 1 presents an idealized structure and dynamics of knowledge production. This diagram represents, on the Experiment side (left column) the laboratory or field operations of an empirical science, where experiments are designed and built, observable effects are generated and measured, and the experimental data bank is assembled. On the Theory side (right column), the diagram represents the theoretical work of statistical analysis, interpretation and (hopefully) understanding according to accepted patterns. If necessary, new hypotheses (including whole new theories) are formulated, motivating the design of new experiments. Theory and experiment constitute a double feed-back cycle making it clear that the design of experiments is guided by the existing theory and its interpretation, which, in turn, must be constantly checked, adapted or modified in order to cope with the observed experiments. The whole system constitutes an autopoietic unit, as seen in Krohn and Küppers (1990, p.214):

> *"The idea of knowledge as an eigensolution of an operationally closed combination between argumentative and experimental activities attempts to answer the initially posed question of how the construction of knowledge binds itself to its construction in a new way. The coherence of an eigensolution does not refer to an objectively given reality but follows from the operational closure of the construction. Still, different decisions on the selection of couplings may lead to different, equally valid eigensolutions. Between such different solutions no reasonable choice is possible unless a new operation of knowledge is constructed exactly upon the differences of the given solutions. But again, this frame of reference for explicitly relating different solutions to each other introduces new choices with respect to the coupling of operations and explanations. It does not reduce but enhances the dependence of knowledge on decisions. On the other hand, the internal restrictions imposed by each of the chosen couplings do not allow for any arbitrary construction of results. Only few are suitable to mutually serve as inputs in a circular operation of knowledge."*

1.5   Sharp Statistical Hypotheses

Statistical science is concerned with inference and application of probabilistic models. From what has been presented in the preceding sections, it becomes clear what the role of Statistics in scientific research is, at least in the ConsTh view of scientific research: Statistics has a dual task, to be performed both in the Theory and the Experiment sides of the diagram in Figure 1:

Experiment		Theory
Operation- ⇐ Experiment ⇐ Hypotheses		
alization design formulation		
⇓ ⇑		
Effects True/False Creative		
observation eigen-solution interpretation		
⇓ ⇑		
Data Mnemetic Statistical		
acquisition ⇒ explanation ⇒ analysis		
Sample space		Parameter space
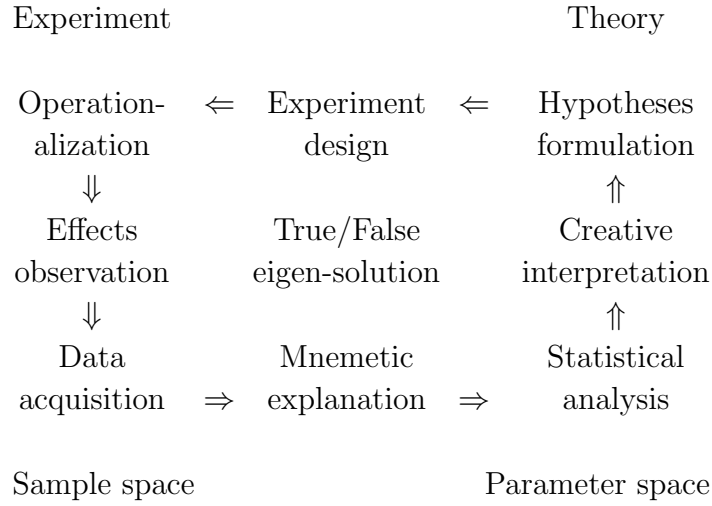
Figure 1: Scientific production diagram.

- At the Experiment side of the diagram, the task of statistics is to make probabilistic statements about the occurrence of pertinent events, i.e. describe probabilistic distributions for what, where, when or which events can occur. If the events are to occur in the future, these descriptions are called predictions, as is often the case in the natural sciences. It is also possible (more often in social sciences) to deal with observations related to past events, that may or may not be experimentally generated or repeated, imposing limitations to the quantity and/or quality of the available data. Even so, the habit of calling this type of statement "predictive probabilities" will be maintained.

- At the Theory side of the diagram, the role of statistics is to measure the statistical support of hypotheses, i.e. to measure, quantitatively, the hypotheses plausibility or possibility in the theoretical framework where they were formulated, given the observed data. From the material presented in the preceding sections, it is also clear that, in this role, statistics is primarily concerned with measuring the statistical support of sharp hypotheses, for hypotheses sharpness (precision or discreteness) is an essential attribute of eigen-solutions.

Let us now examine how well the traditional statistical paradigms, and in contrast the FBST, are able to take care of this dual task. In order to examine this question, the first step is to distinguish what kind of probabilistic statements can be made. We make use of tree statement categories: Frequentist, Epistemic and Bayesian:

Frequentist probabilistic statements are made exclusively on the basis of the frequency

of occurrence of an event in a (potentially) infinite sequence of observations generated by a random variable.

Epistemic probabilistic statements are made on the basis of the epistemic status (degree of belief, likelihood, truthfulness, validity) of an event from the possible outcomes generated by a random variable. This generation may be actual or potential, that is, may have been realized or not, may be observable or not, may be repeated an infinite or finite number of times.

Bayesian probabilistic statements are epistemic probabilistic statements generated by the (in practice, always finite) recursive use of Bayes formula:

$$p_n(\theta) \propto p_{n-1}(\theta) p(x_n | \theta) \ .$$

In standard models, the parameter θ, a non observed random variable, and the sample x, an observed random variable, are related through their joint probability distribution, $p(x, \theta)$. The prior distribution, $p_0(\theta)$, is the starting point for the Bayesian recursion operation. It represents the initial available information about θ. In particular, the prior may represent no available information, like distributions obtained via the maximum entropy principle, see Dugdale (1996) and Kapur (1989). The posterior distribution, $p_n(\theta)$, represents the available information on the parameter after the n-th "learning step", in which Bayes formula is used to incorporate the information carried by observation x_n. Because of the recursive nature of the procedure, the posterior distribution in a given step is used as prior in the next step.

Frequentist statistics dogmatically demands that all probabilistic statements be frequentist. Therefore, any direct probabilistic statement on the parameter space is categorically forbidden. Scientific hypotheses are epistemic statements about the parameters of a statistical model. Hence, frequentist statistics can not make any direct statement about the statistical significance (truthfulness) of hypotheses. Strictly speaking it can only make statements at the Experiment side of the diagram. The frequentist way of dealing with questions on Theory side of the diagram, is to embed them some how into the Experiment side. One way of doing this is by using a construction in which the whole data acquisition process is viewed as a single outcome of an imaginary infinite meta random process, and then make a frequentist statement, on the meta process, about the frequency of unsatisfactory outcomes of some incompatibility measure of the observed data bank with the hypothesis. This is the classic (and often forgotten) rationale used when stating a p-value. So we should always speak of the p-value of the data bank (not of the hypothesis). The resulting conceptual confusion and frustration (for most working scientists) with this kind of convoluted reasoning is captured by a wonderful parody of Galileo's dialogues in Rouanet et al. (1998).

A p-value is the probability of getting a sample that is more extreme than the one we got. We should therefore specify which criterion is used to define what we mean by more

extreme, i.e., how do we order the sample space, and usually there are several possible criteria to do that, for examples, see Pereira and Wechsler (1993).
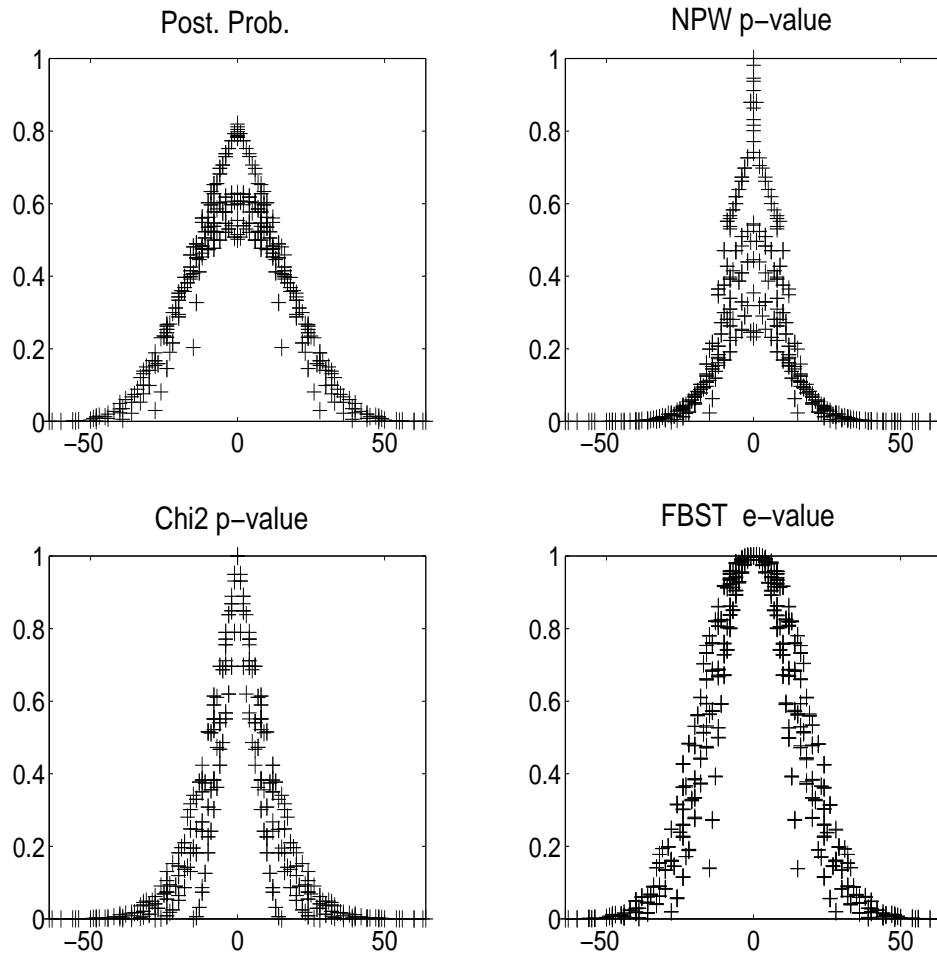
Figure 2: Independence Hypothesis, n=16.

Figure 2 compares four statistics, namely, orthodox Bayesian posterior probabilities, Neyman-Pearson-Wald (NPW) p-values, Chi-square approximate p-values, and the FBST evidence value in favor of H. In this example H is the independence hypothesis in a 2×2 contingency table, for sample size $n = 16$, see section A1 and B1. The horizontal axis shows the "diagonal asymmetry" statistics (difference between the diagonal products). The statistics D is an estimator of an unnormalized version of Person's correlation coefficient, ρ. For detailed explanations, see Irony et al. (1995, 2000), Stern and Zacks (2002) and Madruga, Pereira and Stern (2003).

$$ D = x_{1,1}x_{2,2} - x_{1,2}x_{2,1} \quad , \quad \rho = \frac{\sigma_{1,2}}{\sqrt{\sigma_{1,1}\sigma_{2,2}}} = \frac{\theta_{1,1}\theta_{2,2} - \theta_{1,2}\theta_{2,1}}{\sqrt{\theta_{1,1}\theta_{1,2}\theta_{2,1}\theta_{2,2}}} \ . $$

Samples that are "perfectly compatible with the hypothesis", that is, having no asymmetry, are near the center of the plot, with increasingly incompatible samples to the sides.

The envelope curve for the resulting FBST e-values, to be commented later in this section, is smooth and therefore level at its maximum, where it reaches the value 1.

In contrast the envelope curves for the p-values take the form of a cusp, i.e. a pointed curve, that is broken (non differentiable) at its maximum, where it also reaches the value one. The acuteness of the cusp also increases with increasing sample size. In the case of NPW p-values we see, at the top of the cusp, a "ladder" or "spike", with several samples with no asymmetry, but having different outcome probabilities, "competing" for the higher p-value.

This is a typical collateral effect of the artifice that converts a question about the significance of H, asking for a probability in the parameter space as an answer, into a question, conditional on H being truth, about the outcome probability of the observed sample, offering a probability in the sample space as an answer. This qualitative analysis of the p-value methodology gives us an insight on typical abuses of the expression *"increase sample size to reject"*. In the words of I.J. Good (1983, p.135):

> *"Very often the statistician doesn't bother to make it quite clear whether his null hypothesis is intended to be sharp or only approximately sharp....*
>
> *It is hardly surprising then that many Fisherians (and Popperians) say that - you can't get (much) evidence in favor of the null hypothesis but can only refute it."*

In Bayesian statistics we are allowed to make probabilistic statements on the parameter space, and also, of course, in the sample space. Thus it seems that Bayesian statistics is the right tool for the job, and so it is! Nevertheless, we must first examine the role played by DecTh in orthodox Bayesian statistics. Since the pioneering work of de Finetti, Savage and many others, orthodox Bayesian Statistics has developed strong and coherent foundations grounded on DecTh, where many basic questions could be successfully analyzed and solved.

This foundations can be stratified in two layers:

- In the first layer, DecTh provides a coherence system for the use of probability statements, in the sense of Finetti (1974, 1981). In this context, the FBST use of probability theory is fully compatible with DecTh, as shown in Madruga et al. (2001).

- In the second layer, DecTh provides an epistemological framework for the interpretation of statistical procedures. The FBST logical properties open the possibility of using and benefiting from alternative epistemological settings such as ConsTh. Hence, DecTh does not have to be "the tool for all trades".

We claim that, in the specific case of statistical procedures for measuring the support (significance tests) for sharp scientific hypotheses, ConsTh provides a more adequate epistemological framework than DecTh. This point is as important as it is subtle. In order

to understand it let us first remember the orthodox paradigm, as it is concisely stated in Dubins and Savage (1965, 12.8, p.229,230). In a second quote, from Savage (1954, 16.3, p.254) we find that sharp hypotheses, even if important, make little sense in this paradigm, a position that is accepted throughout decision theoretic Bayesian statistics, as can also be seen in Levi (1974) and Maher et al. (1993).

> *"Gambling problems in which the distributions of various quantities are prominent in the description of the gambler's fortune seem to embrace the whole of theoretical statistics according to one view (which might be called the decision-theoretic Bayesian view) of the subject.*

> *...From the point of view of decision-theoretic statistics, the gambler in this problem is a person who must ultimately act in one of two ways (the two guesses), one of which would be appropriate under one hypothesis (H_0) and the other under its negation (H_1).*

> *...Many problems, of which this one is an instance, are roughly of the following type. A person's opinion about unknown parameters is described by a probability distribution; he is allowed successively to purchase bits of information about the parameters, at prices that may depend (perhaps randomly) upon the unknown parameters themselves, until he finally chooses a terminal action for which he receives an award that depends upon the action and parameters."*

> *"I turn now to a different and, at least for me, delicate topic in connection with applications of the theory of testing. Much attention is given in the literature of statistics to what purport to be tests of hypotheses, in which the null hypothesis is such that it would not really be accepted by anyone. ... extreme (sharp) hypotheses, as I shall call them...*

> *...The unacceptability of extreme (sharp) null hypotheses is perfectly well known; it is closely related to the often heard maxim that science disproves, but never proves, hypotheses, The role of extreme (sharp) hypotheses in science and other statistical activities seems to be important but obscure. In particular, though I, like everyone who practice statistics, have often "tested" extreme (sharp) hypotheses, I cannot give a very satisfactory analysis of the process, nor say clearly how it is related to testing as defined in this chapter and other theoretical discussions."*

As it is clearly seen, in the DecTh framework we speak about the betting odds for "the hypothesis wining on a gamble taking place in the parameter space". But since sharp hypotheses are zero (Lebesgue) measure sets, our betting odds must be null, i.e. sharp hypotheses must be (almost surely) false. If we accept the ConsTh view that an important class of hypotheses concern the identification of eigen-solutions, and that those are ontologically sharp, we have a paradox!

From these considerations it is not surprising that frequentist and DecTh orthodoxy consider sharp hypotheses, at best as anomalous crude approximations used when the scientist is incapable of correctly specifying error bounds, cost, loss or utility functions, etc., or then just consider them to be *"just plain silly"*. In the words of D.Williams (2002, p.234):

> *"Bayesian significance of sharp hypothesis: a plea for sanity: ...It astonishes me therefore that some Bayesian now assign non-zero prior probability that a sharp hypothesis is exactly true to obtain results which seem to support strongly null hypotheses which frequentists would very definitely reject. (Of course, it is blindingly obvious that such results must follow)."*

But no matter how many times statisticians reprehend scientist for their sloppiness and incompetence, they keep formulating sharp hypotheses, as if they where magnetically attracted to them. From the ConsTh plus FBST perspective they are, of course, just doing the right thing!

Decision theoretic statistics has also developed methods to deal with sharp hypotheses, posting sometimes a scary caveat emptor for those willing to use them. The best known of such methods are Jeffreys' tests, based on Bayes Factors that assign a positive prior probability mass to the sharp hypothesis. This positive prior mass is supposed to work like a handicap system designed to balance the starting odds and make the game "fair". Out of that we only get new paradoxes, like the well documented Lindley's paradox. In opposition to its frequentist counterpart, this is an "increase sample size to accept" effect, see Shafer (1982).

The FBST e-value or evidence value supporting the hypothesis, $\text{ev}(H)$, was specially designed to effectively evaluate the support for a sharp hypothesis, H. This support function is based on the posterior probability measure of a set called the tangential set, $\overline{T}(H)$, which is a non zero measure set (so no null probability paradoxes), see Pereira and Stern (1999), Madruga et al. (2003) and subsection A1 of the appendix.

Although $\text{ev}(H)$ is a probability in the parameter space, it is also a possibilistic support function. The word *possibilistic* carries a heavy load, implying that $\text{ev}(H)$ complies with a very specific logic (or algebraic) structure, as seen in Darwishe and Ginsberg (1992), Stern (2003, 2004), and subsection A3 of the appendix. Furthermore the e-value has many necessary or desirable properties for a statistical support function, such as:

1- Give an intuitive and simple measure of significance for the hypothesis in test, ideally, a *probability* defined directly in the original or *natural parameter space.*

2- Have an intrinsically geometric definition, independent of any non-geometric aspect, like the particular parameterization of the (manifold representing the) null hypothesis being tested, or the particular coordinate system chosen for the parameter space, i.e., be an *invariant* procedure.

3- Give a measure of significance that is smooth, i.e. *continuous and differentiable*, on the hypothesis parameters and sample statistics, under appropriate regularity conditions of the model.

4- Obey the *likelihood principle* , i.e., the information gathered from observations should be represented by, and only by, the likelihood function.

5- Require *no ad hoc artifice* like assigning a positive prior probability to zero measure sets, or setting an arbitrary initial belief ratio between hypotheses.

6- Be a *possibilistic* support function.

7- Be able to provide a *consistent* test for a given sharp hypothesis.

8- Be able to provide *compositionality* operations in complex models.

9- Be an *exact* procedure, not requiring "large sample" asymptotic approximations.

10- Allow the incorporation of previous experience or expert's opinion via (subjective) *prior distributions*.

For a careful and detailed explanation of the FBST definition, its computational implementation, statistical and logical properties, and several already developed applications, the reader is invited to consult some of the articles in the reference list. Appendix A provides a short review of the FBST, including its definition and main properties.

1.6   Semantic Degradation

In this section some constructivist analyses of dedifferentiation phenomena in social systems are reviewed. If the conclusions in the last section are correct, it is surprising how many times DecTh, sometimes with a very narrow pseudo-economic interpretation, was misused in scientific statistical analysis. The difficulties of testing sharp hypotheses in the traditional statistical paradigms are well documented, and extensively discussed in the literature, see for example the articles in Harlow et al. (1997). We hope the material in this section can help us understand these difficulties as symptoms of problems with much deeper roots. By no means the author is the first to point out the danger of analyses carried out by blind transplantation of categories between heterogeneous systems. In particular, regarding the abuse of economical analyses, Luhmann (1989, p.164) states:

> *"In this sense, it is meaningless to speak of "non-economic" costs. This is only a metaphorical way of speaking that transfers the specificity of the economic mode of thinking indiscriminately to other social systems."*

For a sociological analysis of this phenomenon in the context of science, see for example Fuchs (1996, p.310) and DiMaggio and Powell (1991, p.63):

> *"...higher-status sciences may, more or less aggressively, colonize lower-status fields in an attempt at reducing them to their own First Principles. For particle physics, all is quarks and the four forces. For neurophysiology, consciousness is the aggregate outcome of the behavior of neural networks. For sociobiology, philosophy is done by ants and rats with unusual large brains that utter metaphysical nonsense according to acquired reflexes. In short, successful and credible chains or reductionism usually move from the top to the bottom of disciplinary prestige hierarchies."*

> *"This may explain the popularity of giving an "economical understanding" to processes in functionally distinct areas even if (or perhaps because) this semantics is often hidden by statistical theory and methods based on decision theoretic analysis. This also may explain why some areas, like ecology, sociology or psychology, are (or where) far more prone to suffer this kind of dedifferentiation by semantic degradation than others, like physics."*

Once the forces pushing towards systemic degradation are clearly exposed, we hope one can understand the following corollary of von Foerster famous ethical and aesthetical imperatives:

- Theoretical imperative: Preserve systemic autopoiesis and semantic integrity, for dedifferentiation is in-sanity itself.

- Operational imperative: Chose the right tool for each job: "If you only have a hammer, everything looks like a nail".

1.7   Competing Sharp Hypotheses

In this section we examine the concept of *Competing Sharp Hypotheses*. This concept has several variants, but the basic idea is that a good scientist should never test a single sharp hypothesis, for it would be an unfair faith of the poor sharp hypothesis standing all alone against everything else in the world. Instead, a good scientist should always confront a sharp hypothesis with a competing sharp hypotheses, making the test a fair game. As seen in Good (1983, p.167,135,126):

> *"Since I regard refutation and corroboration as both valid criteria for this demarcation it is convenient to use another term, Checkability, to embrace both processes. I regard checkability as a measure to which a theory is scientific, where checking is to be taken in both its positive and negative senses, confirming and disconfirming."*

> *"...If by the truth of Newtonian mechanics we mean that it is approximately true in some appropriate well defined sense we could obtain strong evidence*

> *that it is true; but if we mean by its truth that it is exactly true then it has already been refuted."*

> *"...I think that the initial probability is positive for every self-consistent scientific theory with consequences verifiable in a probabilistic sense. No contradiction can be inferred from this assumption since the number of statable theories is at most countably infinite (enumerable)."*

> *"...It is very difficult to decide on numerical values for the probabilities, but it is not quite so difficult to judge the ratio of the subjective initial probabilities of two theories by comparing their complexities. This is one reason why the history of science is scientifically important."*

The competing sharp hypotheses argument does not directly contradict the epistemological framework presented in this chapter, and it may be appropriate under certain circumstances. It may also mitigate or partially remediate the paradoxes pointed out in the previous sections when testing sharp hypotheses in the traditional frequentist or orthodox Bayesian settings. However, the author does not believe that having competing sharp hypotheses is neither a necessary condition for good science practice, nor an accurate description of science history.

Just to stay with Good's example, let us quickly examine the very first major incident in the tumultuous debacle of Newtonian mechanics. This incident was Michelson's experiment on the effect of "aethereal wind" over the speed of light, see Michelson and Morley (1887) and Lorentz et al. (1952). A clear and lively historical account to this experiment can be found in Jaffe (1960). Actually Michelson found no such effect, i.e. he found the speed of light to be constant, invariant with the relative speed of the observer. This result, a contradiction in Newtonian mechanics, is easily explained by Einstein's special theory of relativity. The fundamental difference between the two theories is their symmetry or invariance groups: Galileo's group for Newtonian mechanics, Lorentz' group for special relativity. A fundamental result of physics, Noether's Theorem, states that for every continuous symmetry in a physical theory, there must exist an invariant quantity or conservation law. For detail the reader is refered to Byron and Fuller (1969, V-I, Sec. 2.7), Doncel et al. (1987), Gruber et al. (1980-98), Houtappel et al. (1965), French (1968), Landau and Lifchitz (1966), Noether (1918), Wigner (1970), Weyl (1952). Conservation laws are sharp hypotheses ideally suited for experimental checking. Hence, it seems that we are exactly in the situation of competing sharp hypotheses, and so we are today, from a far away historical perspective. But this is a post-mortem analysis of Newtonian mechanics. At the time of the experiment there was no competing theory. Instead of confirming an effect, specified only within an order of magnitude, Michelson found, for his and everybody else's astonishment, an, up to the experiment's precision, null effect.

Complex experiments like Michelson's require a careful analysis of experimental errors, identifying all significant source of measurement noise and fluctuation. This kind of

analysis is usual in experimental physics, and motivates a brief comment on a secondary source of criticism on the use of sharp hypotheses. In the past, one often had to work with over simplified statistical models. This situation was usually imposed by limitations such as the lack of better or more realistic models, or the unavailability of the necessary numerical algorithms or the computer power to use them. Under these limitations, one often had to use minimalist statistical models or approximation techniques, even when these models or techniques were not recommended. These models or techniques were instrumental to provide feasible tools for statistical analysis, but made it very difficult to work (or proved very ineffective) with complex systems, scarce observations, very large data sets, etc. The need to work with complex models, and other difficult situations requiring the use of sophisticated statistical methods and techniques, is very common (and many times inescapable) in research areas dealing with complex systems like biology, medicine, social sciences, psychology, and many other fields, some of them distinguished with the mysterious appellation of "soft" science. A colleague once put it to me like this: "It seems that physics got all the easy problems...".

If there is one area where the computational techniques of Bayesian statistics have made dramatic contributions in the last decades, that is the analysis of complex models. The development of advanced statistical computational techniques like Markov Chain Monte Carlo (MCMC) methods, Bayesian and neural networks, random fields models, and many others, make us hope that most of the problems related to the use of over simplified models can now be overcome. Today good statistical practice requires all statistically significant influences to be incorporated into the model, and one seldom finds an acceptable excuse not to do so; see also Pereira and Stern (2001).

1.8   Final Remarks

It should once more be stressed that most of the material presented in sections 2, 3, 4, and 6 is not new in ConsTh. Unfortunately ConsTh has had a minor impact in statistics, and sometimes provoked a hostile reaction from the ill-informed. One possible explanation of this state of affairs may be found in the historical development of ConsTh. The constructivist reaction to a dogmatic realism prevalent in hard sciences, specially in the XIX and the beginning of the XX century, raised a very outspoken rhetoric intended to make explicitly clear how naive and fragile the foundations of this over simplistic realism were. This rhetoric was extremely successful, quickly awakening and forever changing the minds of those directly interested in the fields of history and philosophy of science, and spread rapidly into many other areas. Unfortunately the same rhetoric could, in a superficial reading, make ConsTh be perceived as either hostile or intrinsically incompatible with the use of quantitative and statistical methods, or leading to an extreme forms of subjectivism.

In ConsTh, or (objective) Idealism as presented in this chapter, neither does one claim to have access to a "thing in itself" or "Ding an sich" in the external environment, see Caygill (1995), as do dogmatic forms of realism, nor does one surrender to solipsism, as do skeptic forms of subjectivism, including some representatives of the subjectivist school of probability and statistics, as seen in Finetti (1974, 1.11, 7.5.7). In fact, it is the role of the external constraints imposed by the environment, together with the internal autopoietic relations of the system, to guide the convergence of the learning process to precise eigensolutions, these being at the end, the ultimate or real objects of scientific knowledge. As stated by Luhmann (1990a, 1995):

> *"...constructivism maintains nothing more than the unapproachability of the external world "in itself" and the closure of knowing - without yielding, at any rate, to the old skeptical or "solipsistic" doubt that an external world exists at all-..."* Luhmann (1990a, p.65).

> *"...at least in systems theory, they (statements) refer to the real world. Thus the concept of system refers to something that in reality is a system and thereby incurs the responsibility of testing its statements against reality."* Luhmann (1995, p.12).

> *"...both subjectivist and objectivist theories of knowledge have to be replaced by the system / environment distinction, which then makes the distinction subject / object irrelevant."* Luhmann (1990a, p.66).

The author hopes to have shown that ConsTh not only gives a balanced and effective view of the theoretical / experimental aspects of scientific research but also that it is well suited (or even better suited) to give the necessary epistemological foundations for the use of quantitative methods of statistical analysis needed in the practice of science. It should also be stressed, according to author's interpretation of ConsTh, the importance of measuring the statistical support for sharp hypotheses. In this setting, the author believes that, due to its statistical and logical characteristics, the FBST is the right tool for the job, and hopes to have motivated the reader to find more about the FBST definition, theoretical properties, efficient computational implementation, and several of the already developed applications, in some of the articles in the reference list. This perspective opens interesting areas for further research. Among them, we mention the following two.

1.8.1   Noether and de Finetti Theorems

The first area for further research has to do with some similarities between Noether theorems in physics, and de Finetti type theorems in statistics. Nother theorems provide invariant physical quantities or conservation laws from symmetry transformation groups of the physical theory, and conservation laws are sharp hypotheses by excellence. In

a similar way, de Finetti type theorems provide invariant distributions from symmetry transformation groups of the statistical model. Those invariant distributions can in turn provide prototypical sharp hypotheses in many application areas. Physics has its own heavy apparatus to deal with the all important issues of invariance and symmetry. Statistics, via de Finetti theorems, can provide such an apparatus for other areas, even in situations that are not naturally embedded in a heavy mathematical formalism, see Feller (1968, ch.7) and also Diaconis (1987, 1988), Eaton (1989), Nachbin (1965) Renyi (1970) and Ressel (1987).

1.8.2   Compositionality

The second area for further research has to do with one of the properties of eigen-solutions mentioned by von Foerster that has not been directly explored in this chapter, namely that eigen-solutions are "composable", see Borges and Stern (2005) and section A4. Compositionality properties concern the relationship between the credibility, or truth value, of a complex hypothesis, H, and those of its elementary constituents, H^j, $j = 1 \ldots k$. Compositionality questions play a central role in analytical philosophy.

According to Wittgenstein (2001, 2.0201, 5.0, 5.32):

- Every complex statement can be analyzed from its elementary constituents.

- Truth values of elementary statement are the results of those statements' truth-functions (Wahrheitsfunktionen).

- All truth-function are results of successive applications to elementary constituents of a finite number of truth-operations (Wahrheitsoperationen).

Compositionality questions also play a central role in far more concrete contexts, like that of reliability engineering, see Birnbaum et al. (1961, 1.4):

> "One of the main purposes of a mathematical theory of reliability is to develop means by which one can evaluate the reliability of a structure when the reliability of its components are known. The present study will be concerned with this kind of mathematical development. It will be necessary for this purpose to rephrase our intuitive concepts of structure, component, reliability, etc. in more formal language, to restate carefully our assumptions, and to introduce an appropriate mathematical apparatus."

In Luhmann (1989, p.79) we find the following remark on the evolution of science that directly hints the importance of this property:

> "After the (science) system worked for several centuries under these conditions it became clear where it was leading. This is something that idealization,

> *mathematization, abstraction, etc. do not describe adequately. It concerns the increase in the capacity of decomposition and recombination, a new formulation of knowledge as the product of analysis and synthesis. In this case analysis is what is most important because the further decomposition of the visible world into still further decomposable molecules and atoms, into genetic structures of life or even into the sequence human/role/action/ action-components as elementary units of systems uncovers an enormous potential for recombination."*

In the author's view, the composition (or re-combination) of scientific knowledge and its use, so relevant in technology development and engineering, can give us a different perspective (perhaps a, bottom-up, as opposed to the top-down perspective in this chapter) on the importance of sharp hypotheses in science and technology practice. It can also provide some insight on the valid forms of iteration of science with other social systems or, in Luhmann's terminology, how science does (or should) "resonate" in human society.

Chapter 2

Language and the Self-Reference Paradox

"If the string is too tight it will snap,
but if it is too loose it will not play."
Siddhartha Gautama.

"The most beautiful thing we can experience is the mysterious.
It is the source of all true art and all science. He to whom
this emotion is a stranger, who can no longer pause to wonder
and stand rapt in awe, is as good as dead: His eyes are closed."
Albert Einstein (1879 - 1955).

2.1   Introduction

In Chapter 1 it is shown how the eigen-solutions found in the practice of science are naturally represented by statistical sharp hypotheses. Statistical sharp hypotheses are routinely stated as natural "laws", conservation "principles" or invariant "transforms", and most often take the form of functional equations, like $h(x) = c$. Chapter 1 also discusses why the eigen-solutions' essential attributes of discreteness (sharpness), stability, and composability, indicate that considering such hypotheses in the practice of science is natural and reasonable. Surprisingly, the two standard statistical theories for testing hypotheses, classical (frequentist p-values) and orthodox Bayesian (Bayes factors), have well known and documented problems for handling or interpreting sharp hypotheses.

These problems are thoroughly reviewed, from statistical, methodological, systemic and epistemological perspectives.

Chapter 1 and appendix A present the FBST, or Full Bayesian Significance Test, an unorthodox Bayesian significance test specifically designed for this task. The mathematical and statistical properties of the FBST are carefully analyzed. In particular, it is shown how the FBST fully supports the test and identification of eigen-solutions in the practice of science, using procedures that take into account all the essential attributes pointed by von Foerster. In contrast to some alternative belief calculi or logical formalisms based on discrete algebraic structures, the FBST is based on continuous statistical models. This makes it easy to support concepts like sharp hypotheses, asymptotic convergence and stability, and these are essential concepts in the representation of eigen-solutions. The same chapter presents cognitive constructivism as a coherent epistemological framework that is compatible with the FBST formalism, and vice-versa. I will refer to this setting as the Cognitive Constructivism plus FBST formalism, or CogCon+FBST framework for short.

The discussion in Chapter 1 raised some interesting questions, some of which we will try to answer in the present chapter. The first question relates to the role and the importance of language in the emergence of eigen-solutions and is discussed in section 2. In answering it, we make extensive use of the William Rasch "two-front war" metaphor of cognitive constructivism, as exposed in Rasch (2000). As explained in section 4, this is the war against dogmatic realism at one front, and against skepticism or solipsism, at the second. The results of the first part of the paper are summarized in section 5. To illustrate his arguments, Rasch uses some ideas of Niels Bohr concerning quantum mechanics. In section 3, we use some of the same ideas to give concrete examples of the topics under discussion. The importance (and also the mystery) related to the role of language in the practice of science was one of the major concerns of Bohr's philosophical writings, see Bohr (1987, I-IV), as exemplified by his famous "dirty dishes" metaphor:

> *"Washing dishes and language can in some respects be compared. We have dirty dishwater and dirty towels and nevertheless finally succeed in getting the plates and glasses clean. Likewise, we have unclear terms and a logic limited in an unknown way in its field of application – but nevertheless we succeed in using it to bring clearness to our understanding of nature."* Bohr (2007).

The second question, posed by Søren Brier, which asks whether the CogCon+FBST framework is compatible with and can benefit from the concepts of Semiotics and Peircean philosophy, is addressed in section 6. In section 7 I present my final remarks.

Before ending this section a few key definitions related to the concept of eigen-solution are reviewed. As stated in Maturana and Varela (1980, p.10), the concept of recurrent state is the key to understand the concept of cognitive domain in an autopoietic system.

"Living systems as units of interaction specified by their conditions of being living systems cannot enter into interactions that are not specified by their organization. The circularity of their organization continuously brings them back to the same internal state (same with respect to the cyclic process). Each internal state requires that certain conditions (interactions with the environment) be satisfied in order to proceed to the next state. Thus the circular organization implies the prediction that an interaction that took place once will take place again. If this does not happen the system maintains its integrity (identity with respect to the observer) and enters into a new prediction. In a continuously changing environment these predictions can only be successful if the environment does no change in that which is predicted. Accordingly, the predictions implied in the organization of the living system are not predictions of particular events, but of classes of inter-actions. Every interaction is a particular interaction, but every prediction is a prediction of a class of interactions that is defined by those features of its elements that will allow the living system to retain its circular organization after the interaction, and thus, to interact again. This makes living systems inferential systems, and their domain of interactions a cognitive domain."

The epistemological importance of this circular (cyclic or recursive) regenerative processes and their eigen (auto, equilibrium, fixed, homeostatic, invariant, recurrent, recursive) -states, both in concrete and abstract autopoietic systems, are further investigated in Foerster and Segal (2001, p.145, 127-128):

"The meaning of recursion is to run through one's own path again. One of its results is that under certain conditions there exist indeed solutions which, when reentered into the formalism, produce again the same solution. These are called "eigen-values", "eigen-functions", "eigen-behaviors", etc., depending on which domain this formation is applied - in the domain of numbers, in functions, in behaviors, etc."

"Objects are tokens for eigen-behaviors. Tokens stand for something else. In exchange for money (a token itself for gold held by one's government, but unfortunately no longer redeemable), tokens are used to gain admittance to the subway or to play pinball machines. In the cognitive realm, objects are the token names we give to our eigen-behavior. When you speak about a ball, you are talking about the experience arising from your recursive sensorimotor behavior when interacting with that something you call a ball. The "ball" as object becomes a token in our experience and language for that behavior which you know how to do when you handle a ball. This is the constructivist's insight into what takes place when we talk about our experience with objects."

Von Foerster also establishes several essential attributes of these eigen-solutions, as quoted in the following paragraph from Foerster (2003c, p.266). These essential attributes can be translated into very specific mathematical properties, that are of prime importance when investigating several aspects of the CogCon+FBST framework.

> *"Eigenvalues have been found ontologically to be discrete, stable, separable and composable, while ontogenetically to arise as equilibria that determine themselves through circular processes. Ontologically, Eigenvalues and objects, and likewise, ontogenetically, stable behavior and the manifestation of a subject's "grasp" of an object cannot be distinguished."*

2.2   Eigen-solutions and Language

Goudsmit (1998, sec.2.3.3, Objects as warrants for eigenvalues), finds an apparent disagreement between the form in which eigen-solutions emerge, according to von Foster and Maturana:

> *"Generally, von Foersters concept of eigenvalue concerns the value of a function after a repeated (iterative) application of a particular operation. ...*
> *This may eventually result in a stable performance, which is an eigenvalue of the observers behavior. The emerging objects are warrants of the existence of these eigenvalues.*
> *... contrary to von Foerster, Maturana considers the consensuality of distinctions as necessary for the bringing forth of objects. It is through the attainment of consensual distinctions that individuals are able to create objects in language. "*

Confirmation for the position attributed by Goudsmit to von Foerster can be found in several of his articles. In Foerster (2003a, p.3), for example, one finds:

> *"... I propose to continue the use of the term 'self-organizing system,' whilst being aware of the fact that this term becomes meaningless, unless the system is in close contact with an environment, which possesses available energy and order, and with which our system is in a state of perpetual interaction, such that it somehow manages to 'live' on the expenses of this environment. ...*
> *... So both the self-organizing system plus the energy and order of the environment have to be given some kind of pre-given objective reality for this view points to function."*

Confirmation for the position attributed by Goudsmit to Maturana can also be found in several of his articles. In Maturana (1988,sec.9.iv), for example, one finds:

> *"Objectivity. Objects arise in language as consensual coordinations of actions that in a domain of consensual distinctions are tokens for more basic coordinations of actions, which they obscure. Without language and outside language there are no objects because objects only arise as consensual coordinations of actions in the recursion of consensual coordinations of actions that languaging is. For living systems that do not operate in language there are no objects; or in other words, objects are not part of their cognitive domains. ... Objects are operational relations in languaging."*

The standpoint of Maturana is further characterized in the following paragraphs from Brier (2005, p.374):

> *"The process of human knowing, is the process in which we, through languaging, create the difference between the world and ourselves; between the self and the non-self, and thereby, to some extent, create the world by creating ourselves. But we do it by relating to a common reality which is in some way before we made the difference between 'the world' and 'ourselves' make a difference, and we do it on some kind of implicit belief in a basic kind of order 'beneath it all'. I do agree that it does not make sense to claim that the world exists completely independently of us. But on the other hand it does not make sense to claim that it is a pure product of our explanations or conscious imagination."*
>
> *"...it is clear that we do not create the trees and the mountains through our experiencing or conversation alone. But Maturana is close to claim that this is what we do."*

In order to understand the above comments, one must realize that Maturana's viewpoints, or at least his rhetoric, changed greatly over time, ranging from the ponderate and precise statements in Maturana and Varela (1980), to some extreme positions assumed in Maturana (1991, p.36-44)), see next paragraph. Maturana must have had in mind the celebrated quote by Albert Einstein at the beginning of this chapter.

> *"Einstein said, and many other scientists have agreed with him, that scientific theories are free creations of the human mind, and he marveled that through them one could understand the universe. The criterion of validation of scientific explanation as operations in the praxis of living of the observer, however, permit us to see how it is that the first reflection of Einstein is valid, and how it is that there is nothing marvelous in that it is so."*

"Scientific explanations arise operationally as generative mechanisms accepted by us as scientists through operations that do not entail or imply any supposition about an independent reality, so that in fact there is no confrontation with one, nor is it necessary to have one even if we believe that we can have one."

"Quantification (or measurements) and predictions can be used in the generation of a scientific explanation but do not constitute the source of its validity. The notions of falsifiability (Popper), verifiability, or confirmation would apply to the validation of scientific knowledge only if this were a cognitive domain that revealed, directly or indirectly, by denotation or connotation, a transcendental reality independent of what the observer does..."

"Nature is an explanatory proposition of our experience with elements of our experience. Indeed, we human beings constitute nature with our explaining, and with our scientific explaining we constitute nature as the domain in which we exist as human beings (or languaging living systems)."

Brier (2005, p.375) further contrasts the standpoint of Maturana with that of von Foerster:

"Von Foerster is more aware of the philosophical demand that to put up a new epistemological position one has to deal with the problem of solipsism and of pure social constructivism."

"The Eigenfunctions do not just come out of the blue. In some, yet only dimly viewed, way the existence of nature and its 'things' and our existence are intertwined in such a way that makes it very difficult to talk about. Von Foerster realizes that to accept the reality of the biological systems of the observer leads into further acceptance about the structure of the environment."

While the position adopted by von Foerster appears to be more realistic or objective, the one adopted by Maturana seems more Idealistic or (inter) subjective. Can these two different positions, which may seem so discrepant, be reconciled? Do we have to chose between an idealistic or a realistic position, or can we rather have both? This is one of the questions we address in the next sections.

In Chapter 1 we used an example of physical eigen-solution (physical invariant) to illustrate the ideas in discussion, namely, the speed of light constant, c. Historically, this example is tied to the birth of Special Relativity theory, and the debacle of classical physics. In this chapter we will illustrate them with another important historical example, namely, the Einstein-Podolsky-Rosen paradox. Historically, this example is tied to questions concerning the interpretation of quantum mechanics. This is one of the main topics of the next section.

2.3 The Languages of Science

At the end of the 19th century, classical physics was the serene sovereign of science. Its glory was consensual and uncontroversial. However, at the beginning of the 20th century, a few experimental results challenged the explanatory power of classical physics. The problems appeared in two major fronts that, from a historical perspective, can be linked to the theories (at that time still non existent) of Special Relativity and quantum mechanics.

At that time, the general perception of the scientific community was that these few open problems could, should and would be accommodated in the framework of classical physics. Crafting sophisticated structural models such as those for the structure of ether (the medium in which light was supposed to propagate), and those for atomic structure, was typical of the effort to circumvent these open problems by artfully maneuvering classical physics. But physics and engineering laboratories insisted, building up a barrage of new and challenging experimental results.

The difficulties with the explanations offered by classical physics not only persisted, but also grew in number and strength. In 1940 the consensus was that classical physics had been brutally defeated, and Relativity and quantum mechanics were acclaimed as the new sovereigns. Let us closely examine some facts concerning the development of quantum mechanics (QM).

One of the first steps in the direction of a comprehensive QM theory was given in 1924 by Louis de Broglie, who postulated the particle-wave duality principle, which states that every moving particle has an associated pilot wave of wavelength $\lambda = h/mv$, where h is Planck's constant and mv is the particle's momentum, i.e., the product of its mass and velocity. In 1926 Erwin Schrödinger stated his wave equation, capable of explaining all known quantic phenomena, and predicting several new ones that where latter confirmed by new experiments. Schrödinger theory is known as Orthodox QM, see Tomonaga (1962) and Pais (1988) for detailed historical accounts. Orthodox QM uses a mathematical formalism based on a complex wave equation, and shares much of the descriptive language of de Broglie's particle-wave duality principle.

There is, however, something odd in the wave-particle descriptions of orthodox QM. When describing a model we speak of each side of a double faced wave-particle entity, as if each side existed by itself, and then inextricably fuse them together in the mathematical formalism. Quoting Cohen (1989, p.87),

> *"Notice how our language shapes our imagination. To say that a particle is moving in a straight line really means that we can set up particle detectors along the straight line and observe the signals they send. These signals would be consistent with a model of the particle as a single chunk of mass moving (back and forth) in accordance with Newtonian particle physics. It is important*

> *to emphasize that we are not claiming that we know what the particle is, but only what we would observe if we set up those particle detectors."*

From Schroedinger's equation we can derive Heisenberg's uncertainty principle, which states that we can not go around measuring everything we want until we pin down every single detail about (the classical entities in our wave-particle model of) reality. One instance of the Heisenberg uncertainty principle states that we can not simultaneously measure a particle position and momentum beyond a certain accuracy. One way of interpreting this instance of the Heisenberg uncertainty principle goes as follows: In classical Newtonian physics our particles are "big enough" so that our measurement devices can obtain the information we need about the particle without disturbing it. In QM, on the other hand, the particles are so small that the measurement operation will always disturb the particle. For example, the light we have to use in order to illuminate the scene, so we can see where the particle is, has to be so strong, relative to the particle size, that it "blows" the particle away changing its velocity. The consequence is that we cannot (neither in practice, nor even in principle) simultaneously measure with arbitrary precision, both the particle's position and momentum. Hence, we have to learn how to tame our imagination and constrain our language.

The need to exercise a strict discipline over what kinds of statements to use was a lesson learned by 20th century physics - a lesson that mathematics had to learn a bit earlier. A classical example from set theory of a statement that cannot be allowed is the Russell's catalog (class, set), defined in Robert (1988, p.x) as:

> *"The 'catalogue of all catalogues not mentioning themselves.' Should one include this catalogue in itself? ... Both decisions lead to a contradiction!"*

Robert (1988) indicates several ways to avoiding this paradox (or antinomy). All of them imply imposing a (very reasonable) set of rules on how to form valid statements. Under any of these rules, Russell's definition becomes an invalid or ill posed statement and, as such, should be disregarded, see Halmos (1998, ch.1 and 2) and Dugundji (1966, ch.1) for introductory texts and Aczel (1988) for an alternative view. Measure theory (of Borel, Lebesgue, Haar, etc.) was a fundamental achievement of 20th century mathematics. It defines measures (notions such as mass, volume and probability) for parts of R^n. However not all parts of R^n are included, and we must refrain of speaking about the measure of inadmissible (non-measurable) sets, see Ulam (1943) for a short article, Kolmogorov and Fomin (1982) for a standard text, and Nachbin (1965) and Bernardo (1993) for extensions pertinent to the FBST formalism. The main subject in Robert (1988) is Non Standard Analysis, a form of extending the languages of both Set Theory and Real Analysis, see the observations in section 6.6 and also Davis (1977, sec.3.4), Goldblatt (1998) and Nelson (1987).

All the preceding examples of mathematical languages have one thing in common: When crafting a specific language, one has to carefully define what kinds of statements are accepted as valid ones. Proper use of the language must be constrained to valid statements. Such constraints are necessary in order to preserve language coherence.

The issue of what kinds of statements should be accepted as valid in QM is an interesting and still subsisting issue, epitomized by the famous debate at the Brussels Solvay conference of 1930 between Niels Bohr and his friend and opponent Albert Einstein. Ruhla (1992, ch.7 and 8) and Baggott (1992, under the topic hidden variables) give very intuitive reviews of the subject, requiring minimal mathematical expertise. Without the details concerning the physics involved, one can describe the debate as: While Bohr suggested very strict rules for admissible statements in QM, Einstein advocated for more amiable ones. In 1935 Einstein, Podolsky and Rosen suggested a "gedankenexperiment", known as the EPR paradox, as a compelling argument supporting Einstein's point of view. D.Bohm, in 1952 and J.Bell, in 1964, contributed to the debate by showing that the EPR paradox could lead to concrete experiments providing a way to settle the debate on empirical grounds. It was only in 1972 that the first EPR experiment could be performed in practice. The observational evidence from these experiments seems to favor Bohr's point of view!

One of today's standard formalisms for QM is Abstract QM, see Hughes (1992) or Chester (1987) for a readable text and Cohen (1989) for a concise and formal treatment. For an alternative formalism based on Niels Bohr's concept of complementarity, see Bohr (1987, I-IV) and Costa and Krause (2004). Other formalisms may also become usefull, see for example Kolmanovskii and Nosov (1986, sec.2.3) and Zubov (1983). Abstract QM, which is very clean and efficient, can be stratified in two layers. In the first layer, all basic calculations are carried out using an algebra of operators in (Rigged) Hilbert spaces. In a second layer, the results of these calculations are interpreted as probabilities of obtaining specific results in physical measurements, see also Rijsbergen (2004). One advantage of using the stratified structure of abstract QM is that it naturally avoids (most of) the danger of forming invalid statements in QM language. Cohen (1989, p.vii) provides the following historical summary:

> *"Historically, ... quantum mechanics developed in three stages. First came a collection of ad hoc assumptions and then a cookbook of equations known as (orthodox) quantum mechanics. The equations and their philosophical underpinning were then collected into a model based on mathematics of Hilbert space. From the Hilbert space model came the abstraction of quantum logics."*

From the above historical comments we draw the following conclusions:

3.1. Each of the QM formalisms discussed in this section, namely, de Broglie wave-particle duality principle, Schrödinger orthodox QM and Hilbert space abstract QM, operates like a language. Maturana stated that objects arise in language. He seems to be right.

3.2. It seems also that new languages must be created (or discovered) to provide us the objects corresponding to the structure of the environment, as stated by von Foerster.

3.3. Exercising a strict discipline concerning what kinds of statements can be used in a given language and context, seems to be vital in many areas.

3.4. It is far from trivial to create, craft, discover, find and/or use a language so that "it works", providing us the "right" objects (eigen-solutions).

3.5. Even when everything looks (for the entire community) fine and well, new empirical evidence can bring our theories down as a castle of cards.

As indicated by an anonymous referee, abstract formalisms or languages do not exist in a vacuum, but sit on top of (or are embedded in) natural (or less abstract) languages. This bring us to the interesting and highly relevant issues of hierarchical language structures and constructive ladders of objects, including interdependence analyses between objects at different levels of such complex structures, see Piaget (1975) for an early reference. For a recent concrete example of the scientific relevance of such interdependences in the field of Psychology, using a Factor Analysis statistical model, see Shedler and Westen (2004, 2005); These issues are among of the main topics addressed in chapter 3 and forthcoming articles.

2.4   The Self-Reference Paradox

The conclusions established in the previous section may look reasonable. In 3.4, however, what exactly are the "right" objects? Clearly, the "right" objects are "those" objects we more or less clearly see and can point at, using as reference language the language we currently use.

There! I have just fallen, head-on, into the quicksands of the self-reference paradox. Don't worry (or do worry), but note this: The self-reference paradox is unavoidable, especially as long as we use English or any other natural human language.

Rasch (2000, p.73,85) has produced a very good description of the self-reference paradox and some of its consequences:

> *"having it both ways seems a necessary consequence... One cannot just have it dogmatically one way, nor skeptically the other... One oscillates, therefore,*

> *between the two positions, neither denying reality nor denying reality's essentially constructed nature. One calls this not idealism or realism, but (cognitive) constructivism."*
>
> *"What do we call this oscillation? We call it paradox. Self - reference and paradox - sort of like love and marriage, horse and carriage."*

Cognitive Constructivism implies a double rejection: That of a solipsist denial of reality, and that of any dogmatic knowledge of the same reality. Rasch uses the "two front war" metaphor to describe this double rejection. Carrying the metaphor a bit further, the enemies of cognitive constructivism could be portrayed, or caricatured, as:

> - Dogmatism despotically requires us to believe in its (latest) theory. Its statements and reasons should be passively accepted with fanatic resignation as infallible truth;
> - Solipsism's anarchic distrust wishes to preclude any established order in the world. Solipsism wishes to transform us into autistic skeptics, incapable of establishing any stable knowledge about the environment in which we live.
> We refer to Caygill (1995, dogmatism) for a historical perspective on the Kantian use of some of the above terms.

Any military strategist will be aware of the danger in the oscillation described by Rasch, which alternately exposes a weak front. The enemy at our strong front will be subjugated, but the enemy at our weak front will hit us hard. Rasch sees a solution to this conundrum, even recognizing that this solution may be difficult to achieve, Rasch (2000, p.85):

> *"There is a third choice: to locate oneself directly on the invisible line that must be drawn for there to be a distinction mind / body (system / environment) in the first place. Yet when one attempts to land on that perfect center, one finds oneself oscillating wildly from side to side, perhaps preferring the mind (system) side, but over compensating to the body (environment) side - or vice versa.*
>
> *The history of post-Kantian German idealism is a history of the failed search for this perfect middle, this origin or neutral ground outside both mind and body that would nevertheless actualize itself as a perfect transparent mind/body within history. Thus, much of contemporary philosophy that both follows and rejects that tradition has become fascinated by, even if trapped in, the mind/body oscillation."*

So, the question is: How do we land on Rasch' fine (invisible) line, finding the perfect center and avoiding dangerous oscillations? This is the topic of the next section.

2.5   Objective Idealism and Pragmatism

We are now ready for a few definitions of basic epistemological terms. These definitions should help us build epistemic statements in a clear and coherent form according to the CogCon+FBST perspective.

> **5.1. Known (knowable) Object:** An actual (potential) eigen-solution of a given system's interaction with its environment. In the sequel, we may use a somewhat more friendly terminology by simply using the term Object.
>
> **5.2. Objective (how, less, more):** Degree of conformance of an object to the essential attributes of an eigen-solution.
>
> **5.3. Reality:** A (maximal) set of objects, as recognized by a given system, when interacting with single objects or with compositions of objects in that set.
>
> **5.4. Idealism:** Belief that a system's knowledge of an object is always dependent on the systems' autopoietic relations.
>
> **5.5. Realism:** Belief that a system's knowledge of an object is always dependent on the environment's constraints.
>
> **5.6. Solipsism, Skepticism:** Idealism without Realism.
>
> **5.7. Dogmatic Realism:** Realism without Idealism.
>
> **5.8. Realistic or Objective Idealism:** Idealism and Realism.
>
> **5.9. "Something in itself":** This expression, used in reference to a specific object, is a marker or label for ill posed statements.

Cog-Con+FBST assumes an objective and idealistic epistemology. Definition 5.9 labels some ill posed dogmatic statements. Often, the description of the method used to access something in itself looks like:

- Something that an observer would observe if the (same) observer did not exist, or

- Something that an observer could observe if he made no observations, or

- Something that an observer should observe in the environment without interacting with it (or disturbing it in any way), and many other equally nonsensical variations.

Some of the readers may not like this form of labeling this kind of invalid statement, preferring to use, instead, a more elaborate terminology, such as "object in parenthesis" (approximately) as object, "object without parenthesis" (approximately) as something in itself, etc. There may be good reasons for doing so, for example, this elaborate language has the advantage of automatically stressing the differences between constructivist and dogmatic epistemologies, see Maturana (1988), Maturana and Poerksen (2004) and Steier (1991). Nevertheless, we have chosen our definitions in agreement with some very pragmatic advice given in Bopry (2002):

> *"Objectivity as defined by a (dogmatic) realist epistemology may not exist within a constructivist epistemology; but, part of making that alternative epistemology acceptable is gaining general acceptance of its terminology. As long as the common use of the terms is at odds with the concepts of an epistemological position, that position is at a disadvantage. Alternative forms of inquiry need to coopt terminology in a way that is consistent with its own epistemology. I suggest that this is not so difficult. The term objective can be taken back..."*

Among the definitions 5.1 to 5.9, definition 5.2 plays a key role. It allows us to say how well an eigen-solution manifests von Foerster's essential attributes, and consequently, how good (objective) is our knowledge of it. However, the degree of objectivity can not be assessed in the abstract, it must be assessed by the means and methods of a given empirical science, namely the one within which the eigen solution is presented. Hence, definition 5.2 relies on an "operational approach", and not on metaphysical arguments. Such an operational approach may be viewed with disdain by some philosophical schools. Nevertheless, for C.S.Peirce it is

"The Kernel of Pragmatism", CP 5.464-465:

> *"Suffice it to say once more that pragmatism is, in itself, no doctrine of metaphysics, no attempt to determine any truth of things. It is merely a method of ascertaining the meanings of hard words and of abstract concepts. ... All pragmatists will further agree that their method of ascertaining the meanings of words and concepts is no other than that experimental method by which all the successful sciences (in which number nobody in his senses would include metaphysics) have reached the degrees of certainty that are severally proper to them today; this experimental method being itself nothing but a particular application of an older logical rule, 'By their fruits ye shall know them'. "*

Definition 5.2 also requires a belief calculus specifically designed to measure the statistical significance, that is, the degree of support of empirical data to the existence of an eigen-solution. In Chapter 1 we showed why confirming the existence of an eigen-solution naturally corresponds to testing a sharp statistical hypotheses, and why the mathematical properties of FBST e-values correspond to the essential attributes of an eigen-solution as stated by von Foerster. In this sense, the FBST calculus is perfectly adequate to support the use of the term Objective and correlated terms in scientific language. Among the most important properties of the e-value mentioned in Chapter 1 and Appendix A, we find:

Continuity: Give a measure of significance that is smooth, i.e. *continuous and differentiable*, on the hypothesis parameters and the sample statistics, under appropriate regularity conditions of the statistical model.

Consistency: Provide a *consistent*, that is, asymptotically convergent significance measure for a given sharp hypothesis.

Therefore, the FBST calculus is a formalism that allow us to assess, continuously and consistently, the objectivity of an eigen-solution, by means of a convergent significance measure, see Chapter 1. We should stress, once more, that achieving comparable goals using alternative formalisms based on discrete algebraic structures may be, in general, rather difficult. Hence, our answer to the question of how to land on Rasch's perfect center is: Replace unstable oscillation for stable convergence!

Any dispute about objectivity (epistemic quality or value of an object of knowledge), should be critically examined and evaluated within this pragmatic program. This program (in the Luhmann's sense) includes the means and methods of the empirical science in which the object of knowledge is presented, and the FBST belief calculus, used to evaluate the empirical support of an object, given the available experimental data.

Even if over optimistic (actually hopelessly utopic), it is worth restating Leibniz' flag of *Calculemus*, as found in Gerhardt (1890, v.7, p.64-65):

> *"Quo facto, quando orientur controversiae, non magis disputatione opus erit inter duos philosophos, quam inter duos Computistas. Sufficiet enim calamos in manus sumere sedereque ad abacos, et sibi mutuo (accito si placet amico) dicere: Calculemus."*

A contemporary translation could read: *Actually, if controversies were to arise, there would be no more need for dispute between two philosophers, rather than between two statisticians. For them it would suffice to reach their computers and, in friendly understanding, say to each other: Let us calculate!*

2.6   The Philosophy of C.S.Peirce

In the previous sections we presented an epistemological perspective based on a pragmatic objective idealism. Objective idealism and pragmatism are also distinctive characteristics of the philosophy of C.S.Peirce. Hence the following question, posed by Søren Brier, that we examine in this section: Is the CogCon+FBST framework compatible with and can it benefit from the concepts of Semiotics and Peircean philosophy?

In Chapter 1 we had already explored the idea that eigen-solutions, as discrete entities, can be named, i.e., become signs in a language system, as pointed by von Foerster in Segal (2001, p.128):

> *"There is an additional point I want to make, an important point. Out of an infinite continuum of possibilities, recursive operations carve out a precise set*

of discrete solutions. Eigen-behavior generates discrete, identifiable entities. Producing discreteness out of infinite variety has incredibly important consequences. It permits us to begin naming things. Language is the possibility of carving out of an infinite number of possible experiences those experiences which allow stable interactions of your-self with yourself."

We believe that the process of recursively "discovering" objects of knowledge, identifying them by signs in language systems, and using these languages to "think" and structure our lives as self-concious beings, is the key for understanding concepts such as signification and meaning. These ideas are explored, in a great variety of contexts, in Bakken and Hernes (2002), Brier (1995), Ceruti (1989), Efran et al. (1990), Eibel-Eibesfeldt (1970), Ibri (1992), Piaget (1975), Wenger et al. (1999), Winograd and Flores (1987) and many others. Conceivably, the key underlying common principle is stated in Brier (2005, p.395):

"The key to the understanding of understanding, consciousness, and communication is that both the animals and we humans live in a self-organized signification sphere which we not only project around us but also project deep inside our systems. Von Uexküll calls it "Innenwelt" (Brier 2001). The organization of signs and the meaning they get through the habits of mind and body follow very much the principles of second order cybernetics in that they produce their own Eigenvalues of sign and meaning and thereby create their own internal mental organization. I call this realm of possible sign processes for the signification sphere. In humans these signs are organized into language through social self-conscious communication, and accordingly our universe is organized also as and through texts. But of course that is not an explanation of meaning."

When studying the organization of self-conscious beings and trying to understand semantic concepts such as signification and meaning, or teleological concepts such as finality, intent and purpose, we move towards domains concerning systems of increasing complexity that are organized as higher hierarchical structures, like the domains of phenomenological, psychological or sociological sciences. In so doing, we leave the domains of natural and technical sciences behind, at least for a moment, see Brent and Bruck (2006) and Muggleton (2006), in last month's issue of *Nature* (March 2006, when this article was written), for two perspectives on future developments.

As observed in Brier (2001), the perception of the objects of knowledge, changes from more objective or realistic to more idealistic or (inter) subjective as we progress to higher hierarchical levels. Nevertheless, we believe that the fundamental nature of objects of knowledge as eigen-solutions, with all the essential attributes pointed out by von Foerster, remains just the same. Therefore, a sign, as understood in the CogCon+FBST framework, always stands for the following triad:

S-1. Some perceived aspects, characteristics, etc., concerning the organization of the autopoietic system.

S-2. Some perceived aspects, characteristics, etc., concerning the structure of the system's environment.

S-3. Some object (discrete, separable, stable and composable eigen-solution based on the particular aspects stated in S-1 and S-2) concerning the interaction of the autopoietic system with its environment.

This triadic character of signs bring us, once again, close to the semiotic theory of C.S.Peirce, offering many opportunities for further theoretical and applied research. For example, we are currently using statistical psychometric analyses in an applied semiotic project for the development of software user interfaces, for related examples see Ferreira (2006). We defer, however, the exploration of these opportunities to forthcoming articles.

In the remainder of this section we focus on a more basic investigation that, we believe, is a necessary preliminary step that must be undertaken in order to acquire a clear conceptual horizon that will assist a sound and steady progress in our future research. The purpose of this investigation is to find out whether the CogCon+FBST framework can find a truly compatible ground in the basic concepts of Peircean philosophy. We proceed establishing a conceptual mapping of the fundamental concepts used to define the Cog-Con+FBST epistemological framework into analogous concepts in Peircean philosophy. Before we start, however, a word of caution: The work of C.S.Peirce is extremely rich, and open to many alternative interpretations. Our goal is to establish the compatibility of CogCon+FBST with one possible interpretation, and not to ascertain reductionist deductions, in any direction.

The FBST is a Continuous Statistical formalism. Our first step in constructing this conceptual mapping addresses the following questions: Is such a formalism amenable to a Perircean perspective? If so, which concepts in Peircean philosophy can support the use of such a formalism?

6.1 Probability and Statistics: The FBST is a probability theory based statistical formalism. Can the probabilistic concepts of the FBST find the necessary support in concepts of Peircean philosophy? We believe that Tychism is such a concept in Peircean philosophy, providing the first element in our conceptual mapping. In CP 6.201 Tychism is defined as:

> *"... the doctrine that absolute chance is a factor of the universe."*

6.2 Continuity: As stated in the previous section, the CogCon+FBST program pursues the stable convergence of the epistemic e-values given by the FBST formalism. The fact that FBST is a belief calculus based on continuous mathematics is essential for its consistency and convergence properties. Again we have to ask: Does the continuity

concept used in the FBST formalism have an analogous concept in Peircean philosophy? We believe that the analogy can be established with the concept of Synechism, thus providing the second element in our conceptual mapping.

In CP 6.169 synechism is defined as:

> *"that tendency of philosophical thought which insists upon the idea of continuity as of prime importance in philosophy and, in particular, upon the necessity of hypotheses involving true continuity."*

6.3 Eigen-Solutions: A key epistemological concept in the CogCon +FBST perspective is the notion of eigen-solution. Although the system theoretic concept of Eigen-solution cannot possibly have an exact correspondent in Peirce philosophy, we believe that Peirce's fundamental concept of "Habit" or "Insistency" offers an adequate analog. Habit, and reality, are defined as:

> *"The existence of things consists in their regular behavior."*, CP 1.411.

> *"Reality is insistency. That is what we mean by 'reality'. It is the brute irrational insistency that forces us to acknowledge the reality of what we experience, that gives us our conviction of any singular."*, CP 6.340.

However, the CogCon+FBST concept of eigen-solution is characterized by von Foerster by several essential attributes. Consequently, in order that the conceptual mapping under construction can be coherent, these characteristics have to be mapped accordingly. In the following paragraphs we show that the essential attributes of sharpness (discreteness), stability and compositionality can indeed be adequately represented.

6.3a Sharpness: The first essential attribute of eigen-solutions stated by von Foerster is discreteness or sharpness. As stated in Chapter 1, it is important to realize that, in the sequel, the term 'discrete', used by von Foerster to qualify eigen-solutions in general, should be replaced, depending on the specific context, by terms such as lower-dimensional, precise, sharp, singular, etc. As physical laws or physical invariants, sharp hypotheses are formulated as mathematical equations.

Can Peircean philosophy offer a good support for sharp hypotheses? Again we believe that the answer is in the affirmative. The following quotations should make that clear. The first three passages are taken from Ibri (1992, p.84-85) and the next two from CP, 1.487 and CP 1.415, see also NEM 4, p.136-137 and CP 6.203.

> *"an object (a thing) IS only in comparison with a continuum of possibilities from which it was selected."*

"Existence involves choice; the dice of infinite faces, from potential to actual, will have the concreteness of one of them."

"...as a plane is a bi–dimensional singularity, relative to a tri-dimensional space, a line in a plane is a topic discontinuity, but each of this elements is continuous in its proper dimension."

" Whatever is real is the law of something less real. Stuart Mill defined matter as a permanent possibility of sensation. What is a permanent possibility but a law?"

"In fact, habits, from the mode of their formation, necessarily consist in the permanence of some relation, and therefore, on this theory, each law of nature would consist in some permanence, such as the permanence of mass, momentum, and energy. In this respect, the theory suits the facts admirably."

6.3b Stability: The second essential attribute of eigen-solutions stated by von Foerster is stability. As stated in Stern (2005), a stable eigen-solution of an operator, defined by a fixed-point or invariance equation, can be found (built or computed) as the limit of a sequence of recursive applications of the operator. Under appropriate conditions (such as within a domain of attraction, for instance) the process convergence and its limiting eigen-solution will not depend on the starting point.

A similar notion of stability for an object-sign complex is given by Peirce. As stated in CP 1.339:

"That for which it (a sign) stands is called its object; that which it conveys, its meaning; and the idea to which it gives rise, its interpretant. The object of representation can be nothing but a representation of which the first representation is the interpretant. But an endless series of representations, each representing the one behind it, may be conceived to have an absolute object at its limit."

6.3c Compositionality: The third essential attribute of eigen-solutions stated by von Foerster is compositionality. As stated in Chapter 1 and Appendix A, compositionality properties concern the relationship between the credibility, or truth value, of a complex hypothesis, H, and those of its elementary constituents, H^j, $j = 1 \ldots k$. Compositionality is at the very heart of any theory of language, see Noeth (1995). As an example of compositionality, see CP 1.366 and CP 6.23. Peirce discusses the composition of forces, that is, how the components are combined using the parallelogram law.

"If two forces are combined according to the parallelogram of forces, their resultant is a real third... Thus, intelligibility, or reason objectified, is what makes Thirdness genuine.".

> *"A physical law is absolute. What it requires is an exact relation. Thus, a physical force introduces into a motion a component motion to be combined with the rest by the parallelogram of forces;".*

In order to establish a minimal mapping, there are two more concepts in CogCon+FBST to which we must assign adequate analogs in Peircean philosophy.

6.4 Extra variability: In Chapter 1 the importance of incorporating all sources of noise and fluctuation, i.e., all the extra variability statistically significant to the problem under study, into the statistical model is analyzed. The following excerpt from CP 1.175 indicates that Peirce's notion of falibillism may be used to express the need for allowing and embracing all relevant (and in practice inevitable) sources of extra variability. According to Peirce, falibilism is *"the doctrine that there is no absolute certainty in knowledge"*.

> *"There is no difficulty in conceiving existence as a matter of degree. The reality of things consists in their persistent forcing themselves upon our recognition. If a thing has no such persistence, it is a mere dream. Reality, then, is persistence, is regularity. ... as things (are) more regular, more persistent, they (are) less dreamy and more real. Fallibilism will at least provide a big pigeon-hole for facts bearing on that theory."*

6.5 - Bayesian statistics: FBST is an Unorthodox Bayesian statistical formalism. Peirce has a strong and unfavorable opinion about Laplace's theory of inverse probabilities.

> *"...the majority of mathematical treatises on probability follow Laplace in results to which a very unclear conception of probability led him. ... This is an error often appearing in the books under the head of 'inverse probabilities'."*
> CP 2.785.

Due to his theory of inverse probabilities, Laplace is considered one of the earliest precursors of modern Bayesian statistics. Is there a conflict between CogCon+FBST and Peirce's philosophy? We believe that a careful analysis of Peirce arguments not only dissipates potential conflicts, but also reinforces some of the arguments used in Chapter 1.

Two main arguments are presented by Peirce against Laplace's inverse probabilities. In the following paragraphs we will identify these arguments and present an up-to-date analysis based on the FBST (unorthodox) Bayesian view:

6.5a - Dogmatic priors vs. Symmetry and Maximum Entropy arguments:

> *"Laplace maintains that it is possible to draw a necessary conclusion regarding the probability of a particular determination of an event based on not knowing*

anything at all [about it]; that is, based on nothing. ... Laplace holds that for every man there is one law (and necessarily but one) of dissection of each continuum of alternatives so that all the parts shall seem to that man to be 'également possibles' in a quantitative sense, antecedently to all information.", CP 2.764.

The dogmatic rhetoric used at the time of Laplace to justify ad hoc prior distributions can easily backfire, as it apparently did for Peirce. Contemporary arguments for the choice of prior distributions are based on MaxEnt formalism or symmetry relations, see Dugdale (1996), Eaton (1989), Kapur (1989) and Nachbin (1965). Contemporary arguments also examine the initial choice of priors by sensitivity analysis, for finite samples, and give asymptotic dissipation theorems for large samples, see DeGroot (1970), Gelman et al. (2003) and Stern (2004). We can only hope that Peirce would be pleased with the contemporary state of the art. These powerful theories have rendered ad hoc priors unnecessary, and shed early dogmatic arguments into oblivion.

6.5b- Assignment of probabilities to (sharp) hypotheses vs. FBST possibilistic support structures:

"Laplace was of the opinion that the affirmative experiments impart a definite probability to the theory; and that doctrine is taught in most books on probability to this day, although it leads to the most ridiculous results, and is inherently self-contradictory. It rests on a very confused notion of what probability is. Probability applies to the question whether a specified kind of event will occur when certain predetermined conditions are fulfilled; and it is the ratio of the number of times in the long run in which that specified result would follow upon the fulfillment of those conditions to the total number of times in which those conditions were fulfilled in the course of experience.", CP 5.169.

In the second part of the above excerpt Peirce expresses a classical (frequentist) understanding of having probability in the sample space, and not in the parameter space, that is, he admits predictive probability statements but does not admit epistemic probability statements. The FBST is a Bayesian formalism that uses both predictive and epistemic probability statements, as explained in Chapter 1. However, when we examine the reason presented by Peirce for adopting this position, in the first part of the excerpt, we find a remarkable coincidence with the arguments presented in Stern (2003, 2004, 2006, 2007) against the orthodox Bayesian methodology for testing sharp hypotheses: The FBST *does not* attribute a *probability* to the theory (sharp hypothesis) being tested, as do orthodox Bayesian tests, but rather a degree of *possibility*. In Stern (2003, 2004, 2006, 2007) we analyze procedures that attribute a probability to a given theory, and came to the exact same conclusion as Pierce did, namely, those procedures are absurd.

6.6 Measure Theory: Let us now return to the Peircean concept of Synechism, to discuss a technical point of contention between orthodox Bayesian statistics and the FBST unorthodox Bayesian approach. The FBST formalism relies on some form of Measure theory, see comments in section 3. De Finetti, the founding father of the orthodox school of Bayesian statistics, feels very uncomfortable having to admit the existence of non-measurable sets when using measure theory in dealing with probabilities, in which valid statements are called events, see Finetti (1975, 3.11, 4.18, 6.3 and appendix). Dubins and Savage (1976, p.8) present similar objections, using the colorful gambling metaphors that are so characteristic of orthodox (decision theoretic) Bayesian statistics. In order to escape the constraint of having non-measurable sets, de Finetti (1975, v.2, p.259) readily proposes a deal: to trade off other standard properties of a measure, like countable (σ) additivity:

> *"Events are restricted to be merely a subclass (technically a σ-ring with some further conditions) of the class of all subsets of the base space. In order to make σ-additivity possible, but without any real reason that could justify saying to one set 'you are an event', and to another 'you are not'."*

In order to proceed with our analysis, we have to search for the roots of de Finetti's argument, roots that, we believe, lay outside de Finetti's own theory, for they hinge on the perceived structure of the continuum. Bell (1998, p.2), states:

> *"the generally accepted set-theoretical formulation of mathematics (is one) in which all mathematical entities, being synthesized from collections of individuals, are ultimately of a discrete or punctate nature. This punctate character is possessed in particular by the set supporting the 'continuum' of real numbers - the 'arithmetical continuum'."*

Among the alternatives to arithmetical punctiform perspectives of the continuum, there are more geometrical perspectives. Such geometrical perspectives allow us to use an arithmetical set as a coordinate (localization) system in the continuum, but the 'ultimate parts' of the continuum, called infinitesimals, are essentially nonpunctiform, i.e. non point like. Among the proponents of infinitesimal perspectives for the continuum one should mention G.W.Leibniz, I.Kant, C.S.Peirce, H.Poincaré, L.E.J.Brouwer, H.Weyl, R.Thom, F.W.Lawvere, A.Robinson, E.Nelson, and many others. Excellent historical reviews are presented in Bell (1998 and 2005), a general view, and Robertson (2001), for the ideas of C.S.Peirce. In the infinitesimal perspective, see Bell (1998, p.3),

> *"any of its (the continuum) connected parts is also a continuum and, accordingly, divisible. A point, on the other hand, is by its nature not divisible, and so (as stated by Leibniz) cannot be part of the continuum."*

In Peirce doctrine of synechism, the infinitesimal geometrical structure of the continuum acts like *" the 'glue' causing points on a continuous line to lose their individual identity."*, see Bell (1998, p.208, 211). According to Peirce, *" The very word continuity implies that the instants of time or the points of a line are everywhere welded together."*

De Finetti's argument on non-measurable sets implicitly assumes that all point subsets of R^n have equal standing, i.e., that the continuum has no structure. Under the arithmetical punctiform perspective of the continuum, de Finetti's objection makes perfect sense, and we should abstain from measure theory or alternative formalisms, as does orthodox Bayesian statistics. This is how Peirce's concept of synechism helps us to overcome a major obstacle (for the FBST) presented by orthodox Bayesian philosophy, namely, the objections against the use of measure theory.

At this point it should be clear that my answer to Brier's question is emphatically affirmative. From Brier's comments and suggestions it is also clear how well he knew the answer when he asked me the question. As a maieutic teacher however, he let me look for the answers my own way. I can only thank him for the invitation that brought me for the first time into contact with the beautiful world of semiotics and Peircean philosophy.

2.7   Final Remarks

The physician Rambam, Moshe ben Maimon (1135–1204) of (the then caliphate of) Cordoba, wrote Shmona Perakim, a book on psychology (medical procedures for healing the human soul) based on fundamental principles exposed by Aristotle in Nicomachean Ethics, see Olitzky (2000) and Rackham (1926). Rambam explains how the health of the human soul depends on always finding the straight path (derech y'shara) or golden way (shvil ha-zahav), at the perfect center between the two opposite extremes of excess (odef) and scarcity (choser), see Maimonides (2001, v.1: Knowledge, ch.2: Temperaments, sec.1,2):

> *"The straight path is the middle one, that is equidistant from both extremes.... Neither should a man be a clown or jokester, nor sad or mourning, but he should be happy all his days in serenity and pleasantness. And so with all the other qualities a man possesses. This is the way of the scholars. Every man whose virtues reflect the middle, is called a chacham... a wise man."*

Rambam explains that a (always imperfect) human soul, at a given time and situation, may be more prone to fall victim of one extreme than to its opposite, and should try to protect itself accordingly. One way of achieving this protection is to offset its position in order to (slightly over-) compensate for an existing or anticipated bias.

At the dawn of the 20th century, humanity had in classical physics a paradigm of science handing out unquestionable truth, and faced the brutality of many totalitarian

states. Dogmatism had the upper hand, and we had to protect ourselves accordingly.

At the beginning of the 21st century we are enjoying the comforts of an hyperactive economy that seems to be blind to the constraints imposed by our ecological environment, and our children are being threatened by autistic alienation through the virtual reality of their video games. It may be the turn of (an apathetic form of) solipsism.

Finally, Rambam warns us about a common mistake: Protective offsets may be a useful precautionary tactic, or even a good therapeutic strategy, but should never be considered as a virtue per se. The virtuous path is the straight path, neither left of it nor right of it, but at the perfect center.

Chapter 3

Decoupling, Randomization, Sparsity, and Objective Inference

"The light dove, that at her free flight cleaves the air,
therefore feeling its resistance, could perhaps imagine
that she would succeed even better in the empty space."

Immanuel Kant (1724-1804),
Critique of Pure Reason (1787, B-8).

Step by step the ladder is ascended.

George Herbert (1593 - 1633),
Jacula Prudentium (1651).

3.1   Introduction

H.von Foerster characterizes "known" objects as eigen-solutions for an autopoietic system, that is, as discrete (sharp), separable (decoupled), stable and composable states of the interaction of the system with its environment. Previous chapters have presented the Full Bayesian Significance Test (FBST) as a mathematical formalism specifically designed to access the support for sharp statistical hypotheses, and have shown that these hypotheses correspond, from a constructivist perspective, to systemic eigen-solutions in the practice of science, as seen in chapter 1. In this chapter, the role and importance of one of these four essential attributes indicated by von Foerster, namely, separation or decoupling, is studied.

Decoupling is the general principle that allows us to understand the world step by step, 'looking' at it a piece at a time, localizing single features, isolating basic components or identifying simple objects, out of the immense complexity of the whole universe. In statistical models, decoupling is often introduced by means of no association assumptions, such as independence, zero covariance, etc. In this context, decoupling relations are sharp statistical hypotheses that can be tested, see for example Stern and Zacks (2002). Decoupling relations in statistical models can also be introduced a priori by means of special Design of Statistical Experiments (DSEs) techniques, the best known of which being randomization.

In chapter 2 the general meaning of the term "Objective" (how, less, more) is defined as the "degree of conformance of an object to the essential attributes of an eigen-solution". One of the common uses of the word objective, as opposed to "subjective", stresses the decoupling or separation of a given systemic eigen-solution, such as an object of a scientific program, from the peculiarities of a second system, such as a specific human observer. It is this restricted meaning, focusing on the decoupling property of systemic eigen-solutions, that justifies the use of the term objective in this chapter's title.

The decoupling principle, and one of its most celebrated examples in Physics, the vibrating chord, are presented in section 2. In the vibrating chord model, a basic linear algebra operation, the eigen-value factorization, is the key to obtain the decoupling operator. In addition, the importance of eigen-solutions and decoupling operations are discussed from a constructivist epistemological perspective. Herein, we shall focus on decoupling operators related to an other basic linear algebra operation, namely, the Cholesky factorization. In section 3 we show how Cholesky factorization can be used to decouple covariance structure models. In section 4, Simpson's paradox and some strategies for DSEs, such as control and randomization, are discussed. These strategies can be used to induce independence relations, that are expressed into the sparsity structure of the model, which can, in turn, be used for efficient decoupling. In section 5, the role of C.S.Peirce in the introduction of control and randomization in DSEs is reviewed from an historical perspective. This revision will help us set the stage for the discussion, in section 6, of a controversial issue: randomization in Bayesian Statistics. In section 7 some epistemological consequences of randomization, are discussed and the underlying themata of constructivism and objective knowledge are revisited.

The Cholesky factorization operator is presented in section 3, in conjunction with the computational concepts of sparse and structured matrices. Covariance structure and Bayesian networks are some of the most basic and widely used statistical models. Therefore, understanding their decoupling properties is important, not only from a computational point of view, but also from the theoretical and a epistemological perspective. Furthermore, one could argue that the usefulness of these statistical models are due exactly to their decoupling properties. Final remarks are presented in section 8.

3.2 The Decoupling Principle

Understanding the entire universe, with all its intricate constituents, relations and inter-connections, can be a daunting task, as stated by Schlick (1979, v.1, p.292):

> *" The most important (of these) difficulties arises from the recognition of the unending linkage of all natural processes one with another. Its effect is that, on an exact view, every occurrence in the world is dependent on every other; the fall of a leaf is ultimately influenced by the motions of the stars, and it would be a task utterly beyond fulfillment to assign its 'cause' with absolute completeness to any given process that we suppose determined down to the last detail. For this purpose we should have to adduce nothing less than all of the circumstances of the universe that have so far occurred.*
>
> *Now fortunately this boundlessness is at once considerably restricted by experience, which teaches us that the reciprocal interdependence of all events in nature is subject to certain easy formulable conditions."*

L.Sadun has written an exceptionally clear book on linear algebra, emphasizing the idea of decoupling, i.e. the strategy of breaking down complicated multivariate systems into simple 'modes', by a suitable change of coordinates, see also Rijsbergen (2004). Sadun (2001, p.1) states the goal of his book as follows:

> *"In this book we cover a variety of linear evolution equations, beginning with the simplest equations in one variable, moving to coupled equations in several variables, and culminating in problems such as wave propagation that involve an infinite number of degrees of freedom. Along the way we develop techniques, such as Fourier analysis, that allow us to decouple the equations into a set of scalar equations that we already know how to solve.*
>
> *The general strategy is always the same. When faced with coupled equations involving variables $x_1, \ldots, x_n$, we define new variables $y_1, \ldots, y_n$. These variables can always be chosen so that the evolution of y_1 depends only of y_1 (and not on $y_2, \ldots, y_n$), the evolution of y_2 depends only of y_2, and so on. To find $x_1(t), \ldots, x_n(t)$ in terms of the initial conditions $x_1(0), \ldots, x_n(0)$, we convert $x(0)$ to $y(0)$, then solve for $y(t)$, then convert to $x(t)$.*

As an example of paramount theoretical and historical importance in Physics, we consider the discrete chord. The chord is kept at tension h, with n particles of mass m at equally spaced positions js, $j = 1 \ldots n$. The extremes of the chord, at positions 0 and $(n + 1)s$, are kept fixed, and $x = [x_1, x_2, \ldots, x_n]'$ denote the particles' vertical
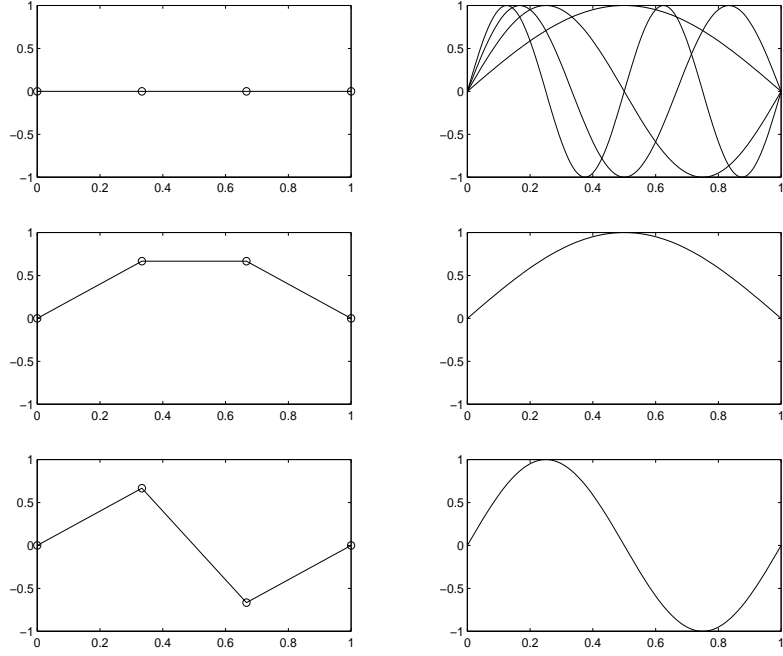
Figure 1: Eigen-Solutions of Continuous and Discrete Chords.

displacements, see French (1974, ch.5 Coupled oscillators and normal modes, p.119-160), Marion (1999, ch.9) and Franklin (1968, ch.7), Figure 1 shows the discrete chord for $n = 2$.

The second order differential equation of classical mechanics, below, privides a linear approximation for the discrete chord system's dynamics:

$$\ddot{x} + Kx = 0 \ , \quad K = w_0^2 \begin{bmatrix} 2 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & \ddots & \vdots \\ 0 & 0 & -1 & \ddots & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & 2 & -1 \\ 0 & 0 & \cdots & 0 & -1 & 2 \end{bmatrix} \ , \quad w_0^2 = \frac{h}{ms} \ .$$

As it is, the discrete chord differential equation is difficult to solve, since the n coordinates of vector x are coupled by matrix K. In the following paragraphs we show how to decouple this differential equation.

Suppose that an orthogonal matrix Q is known to diagonalize matrix K, that is, $Q^{-1} = Q'$, and $Q'KQ = D = \text{diag}(d)$, $d = [d_1, d_2, \ldots, d_n]'$. After pre-multiplying the above differential equation by Q', we obtain the matrix equation

$$Q'(Q\ddot{y}) + Q'K(Qy) = I\ddot{y} + Dy = 0$$

which is equivalent to the n decoupled scalar equations for harmonic oscillators, $\ddot{y}_k + d_k y_k = 0$, in the new 'normal' coordinates, $y = Q'x$. The solution of each harmonic oscillator, as a function of time, t, has the form $y_k(t) = \sin(\varphi_k + w_k t)$, with phase $0 \leq \varphi_k \leq 2\pi$ and angular frequency $w_k = \sqrt{d_k}$.

The columns of matrix Q, the decoupling operator, are the eigenvectors of matrix K, which are, as one can easily check, multiples of the un-normalized vectors z^k. Their corresponding eigenvalues, $d_k = w_k^2$, for $j, k = 1 \ldots n$, are given by

$$z_j^k = \sin\left(\frac{jk\pi}{n+1}\right) \quad , \quad w_k = 2w_0 \sin\left(\frac{k\pi}{2(n+1)}\right) \quad .$$

The decoupled modes of oscillation, for $n = 2$, are depicted in Figure 1. They are called 'normal' modes in physics, 'standing' modes in engineering, and eigen-solutions in mathematics. The discrete chord with n particles will have n normal modes, and the limit case, $n \to \infty$, is called the continuous chord. The normal modes of the continuous chord are given by trigonometric functions, the first few of which are depicted in Figure 1. They are also called 'standing' waves or eigen-functions of the chord, and constitute the basis of Fourier analysis.

In either the discrete or the continuous chord, we can 'excite', i.e. give energy or 'put in motion', one of the normal modes, without affecting any other normal mode. This is the physical meaning of decoupling, i.e. to have 'separate' eigen-solutions. Since the differential equation describing the system is linear, distinct normal modes can also be superposed. This is called the 'superposition' principle, which renders the compositionality rule for the eigen-solutions of the chord.

In the original coordinate system, x, coupling made it hard to follow the system's evolution. In the normal coordinate system, y, based on the system's eigen-solutions, decoupling and superposition made it easier to understand the system behavior. But are these eigen-solutions "just" a formal basis for an alternative coordinate system, or do they represent "real objects" within the system under study?

Obviously, this is not a mathematical or physical question, but rather an epistemological one. From a constructivist perspective, we can consider these eigen-solutions "objectively known" entities in the system. Nevertheless, the meaning of the term objective in a constructivist epistemology is distinct from its meaning in a dogmatic realist epistemology, as explained in Stern (2006b, 2007a,b).

From a constructivist perspective, systemic eigen-solutions can be identified and "named" by an observer. Indeed, the eigen-solutions of the vibrating chord have been identified and named thousands of years before mankind knew anything about differential equations. The eigen-values of the chord are known in music as the 'fundamental tone' and its 'higher harmonics', and constitute the basis for all known musical systems, see Benade (1992).

The linear model for the vibrating chord is a paradigmatic example of the fact that, despite the simplicity to understand and manipulate, linear models often give excellent approximations for complex systems. Also, since linear operators are represented by matrices in standard matrix algebra, the importance of certain matrix operations in the decoupling of such models should not be surprising at all. In the vibrating chord model, the eigen-value factorization, $K = QDQ'$, was the key to obtain the decoupling operator, Q. The eigen-value factorization plays the same role in many important statistical procedures, such as spectral analysis of time series, wavelet signal analysis, and kernel methods.

Related operations of linear algebra, like Singular Value Decomposition, SVD, and Nonnegative Matrix Factorizations, NNMF, are important in principal components analysis and latent structure models, see for example Bertsekas and Tsitsiklis (1989), Censor and S.A.Zenios (1998), Cichocki et al. (2006), Dhillon and Sra (2005) and Hoyer (2004). Distinct decoupling operators have distinct characteristics, relying upon stronger or weaker structural properties of the model, requiring more or less computational work, and having different capabilities for handling sparse data.

In this chapter, we will be mainly interested in the decoupling of statistical models. More precisely, we shall focus on decoupling methods related to an important basic linear algebra operation, namely, the Cholesky factorization. In the next section we show how Cholesky factorization can be used to decouple covariance structure statistical models.

The decoupling principle emerges, sometimes with different denominations, in virtually every area of the hard sciences. In Systems Theory and Mathematical Programming, for example, it arises under the name of Decomposition Methods. In the optimization of large systems, for example, there are two basic approaches to decomposition:

- High level methods focus on the underlying structure of the optimization problems. High level decomposition strategies replace the original large or complex problem by several hierarchically interconnected small or simple optimization problems, see for example Geoffrion (1972), Lasdon (1970) and Wismer (1971).

- Low level methods look at the matrix representation of the optimization problems. Low level decomposition strategies benefit from tailor made computational linear algebra subroutines to take advantage of the underlying sparse matrix structure. Some of these techniques are discussed in the next section.

3.3   Covariance Structure Models

Covariance structure, multivariate regression, Kalman filter and several other related linear statistical models are widely used in the practice of science. They provide a powerful analytical tool in which the association, coupling or dependence between multiple variables

is represented by covariance matrices, as briefly noted in the next paragraphs. These models are simple to manipulate and interpret, and can be implemented using efficient computational algorithms capable of handling millions of (sparsely coupled) variables. In this and the next sections, it is shown how such desirable characteristics of covariance models ultimately rely upon some basic properties of its decoupling operators.

Given a (vector) random variable, x, its covariance matrix, V, is defined as the expected square distance to its expected (mean) value, β, that is,

$$\beta = E(x) , \quad V = \mathrm{Cov}(x) = E((x - \beta) \otimes (x - \beta)') .$$

The diagonal elements, or variances, $\mathrm{Var}(x_i) = V_{i,i}$, give the most usual scalar measure of error, dispersion or uncertainty used in statistics, while the off diagonal elements, $\mathrm{Cov}(x_i, x_j) = V_{i,j}$, give a measure of association between two scalar random variables, x_i and x_j, see Hocking (1985) for a general reference.

Also recall that since the expectation operator, E, is linear, that is, $E(Ax + b) = AE(x) + b$ for any random vector x, matrix A and vector b, we have

$$\mathrm{Cov}(Ax + b) = A\mathrm{Cov}(x)A' .$$

The standard deviation, $\sigma_i = \sqrt{V_{i,i}}$, is a dispersion measure given in the same unit as x, and the correlation, $C_{i,j} = V_{i,j}/\sigma_i\sigma_j$, is a measure of association normalized in the $[-1, 1]$ interval.

As it is usual in the covariance structure literature, we can write a covariance matrix as $V(\gamma) = \sum \gamma_t G^t$, in which the matrices G^t constitute a basis for the space of symmetric matrices of dimension $n \times n$, see Lauretto et al. (2002). For example, for dimension $n = 4$,

$$V(\gamma) = \sum_{t=1}^{10} \gamma_t\, G^t \;=\; \begin{bmatrix} \gamma_1 & \gamma_5 & \gamma_7 & \gamma_8 \\ \gamma_5 & \gamma_2 & \gamma_9 & \gamma_{10} \\ \gamma_7 & \gamma_9 & \gamma_3 & \gamma_6 \\ \gamma_8 & \gamma_{10} & \gamma_6 & \gamma_4 \end{bmatrix} .$$

Using the above notation, we can easily express hypotheses concerning structural properties, including sparsity patterns, in the standard form of vector functional equations, $h(\beta, \gamma) = 0$. Details on how to use the FBST to test such general hypotheses in some particular settings can be found in Lauretto et al. (2002).

Once we have established the structural properties of the model, we can estimate the parameters β and γ accordingly. Following the general line of investigation adopted herein, a question that arises naturally is: How can we decouple the estimated model?

One possible answer to this question can be given in terms of the Cholesky factorization, $LL' = V$ where L is lower triangular. Such a factorization is available for any full rank symmetric matrix V, as shown in Golub and van Loan (1989). Let $V = LL'$ be the

Cholesky factorization of the covariance matrix, V, and let us consider the transformation of variables $y = L^{-1}x$, or $x = Ly$. The covariance matrix of the new variables can be computed as $\text{Cov}(y) = L^{-1}VL^{-t} = L^{-1}LL'L^{-t} = I$. Hence, the transformed model has been decoupled, i.e., has uncorrelated random components.

Let us consider a simple numerical example of Cholesky factorization:

$$
V = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 2 & 0 & 0 \\ 0 & 0 & 4 & 4 \\ 0 & 0 & 4 & 8 \end{bmatrix} \ , \quad L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 2 & 2 \end{bmatrix} \ , \quad V = LL' \ .
$$

This example of Cholesky factorization has some peculiarities: The matrix V is *sparse*, i.e., it has several zero elements. In contrast, a matrix with few or no zero elements is said to be *dense*. Matrix V in the example is also *structured*, i.e., the zeros are arraged in a nice pattern, in this example, a 2×2 off diagonal block. In this example, the Cholesky factor, $L \,|\, LL' = V$, preserves the sparsity and structure of V, that is, no position with a zero in V is *filled* with a non-zero in L. A factorization (or ellimination) resulting in no fill in is called *perfect*. Perfect eliminations are not always possible, however, there are several techniques that can be used to obtain sparse (and structured) Cholesky factorizations in which the fill in is minimized, that is, the sparsity of the Cholesky factor is maximized. Pertinent references on sparse factorizations include Blair and B.Peyton (1993), Bunch and D.J.Rose (1976) George et al. (1978, 1981, 1989, 1993), Golumbic (1980), Pissanetzky (1984), Rose (1972), Rose and Willoughby (1972), Stern (1992,1994), Stern and Vavasis (1993,1994) and van der Vorst and van Dooren (1990).

Large models may have millions of sparsely coupled variables. A sparse and structured factorization of such a model gives a 'simple' decoupling operator, L. This is a matter of vital importance when designing efficient computational procedures. In practice, large models can only be computed with the help of these techniques. An other important class of statistical models, Bayesian Networks, relies on sparse factorization techniques that, from an abstract graph theoretical perspective, are almost identical to sparse Cholesky factorization, see for example Lauritzen (2006) and Stern (2006a, sec.9-11).

In the next section we continue to examine the role of covariance, or more general forms of association, in statistical modeling. On particular, we examine some situations leading to spurious associations, destroying a model's presumed sparsity and structure. In the following sections we review, from an historical and epistemological perspective, some techniques of Design of Statistical Experiments (DSE), used to induce (no) association relations in statistical models. These relations translate into sparsity and structural patterns that, in turn, can be used by efficient factorization algorithms.

3.4 Simpson's Paradox and the Control of Confounding Variables

Lindley (1991, p.47-48) illustrates Simpson's paradox with a medical trial example. From 80 patients in the study, 40 received treatment, T, and 40 received a placebo with no effect, NT. Some patients recovered from their illness, R, and some did not, NR. The recovery rates, R%, are given in Table 1, where the experimental data is shown, both in aggregate form for All patients, and separated or disaggregated according to Sex. Looking at the table one concludes that the treatment is bad for either male or female patients, but good for all of them together! This is the Simpson's Paradox: The association between two variables, T and R in Lindley's example, is reversed if the data is aggregated / disaggregated over a *confounding* variable, Sex in Lindley's example.

Table 1: Simpson's Paradox.

Sex	T	R	NR	Tot	R%
All	T	20	20	40	50%
All	NT	16	24	40	40%
Male	T	18	12	30	60%
Male	NT	7	3	10	70%
Fem	T	2	8	10	20%
Fem	NT	9	21	30	30%

Lindley provides the following scenario for the situation illustrated by this example: The physician responsible for the experiment did not trust the treatment and also was aware that the illness under study affects females most severely. Hence, he decided to try it mainly on males, who would probably recover anyway. This illustrates the general Simpson's paradox situation, generated by the association of the confounding variable with both the explained and one (or more) of the explaining variables. Additional references on several aspects related to the Simpson paradox include Blyth (1972), Cobb (1998), Good and Mittal (1987), Gotzsche (2002), Greenland et al. (1999, 2001), Heydtmann (2002), Hinkelmann (1984), Pearl (2004) and Reintjes et al. (2000).

The obvious question then is: How can we design a statistical experiment in order to avoid spurious associations?

Two strategies are self-evident:

1. Control possible confounding variables in order to impose some form of invariance (constancy, equality) in the experiment, or

2. Measure possible confounding variables so that the relevant ones can be included in the statistical model.

The simplest form of the first strategy would be to test the treatment in a set of 'clones', individuals that are, using the words of Fisher (1966, sec.9, Randomization; the Physical Basis of Validity of the Test, p.17-19),

"exactly alike, in every respect except that to be tested",

This strategy, however, is too strict. Even if feasible, the conclusions of the study would only apply to the 'clone population', not to individuals from a population with natural variability.

A more general form of the first strategy in known as blocking, defined in Box et al. (1978, p.102-103, Sec.4.3, Blocking and Randomization) as:

> *"The device of pairing observations is a special case of 'blocking' that has important applications in many kinds of experiments. A block is a portion of the experimental material (the two shoes of one boy in this example) that is expected to be more homogeneous than the aggregate (all shoes of all the boys). By confining treatment comparisons within such blocks, greater precision can often be obtained."*

Blocking is a very important strategy in the design of statistical experiments (DSEs), used to increase, whenever possible, the precision of the study's conclusions.

As for the second strategy, it looks a sure thing! No statistician would ever refuse more information, in a larger and richer data bank.

Nevertheless, we have to ask whether we want to control and/or measure SOME of the possibly confounding variables, i.e. those perceived as the most important or even those we are aware of, or ALL of them?

Keeping everything under control in a statistical experiment (or in life in general) constitutes, in the words of Fisher,

> *"a totally impossible requirement in our example, and equally in all other forms of experimentation"*.

Not only the cost and complexity of trying to do so for a very large set of variables would be prohibitive in any practical circumstance, but also

> *"it would be impossible to present an exhaustive list of such possible differences (variables) appropriate for any one kind of experiment, because the uncontrolled causes which may influence the result are always strictly innumerable"*.

Modern theory of DSEs offers a way out of this conundrum that, in its most concise form, see Box et al. (1978, p.102-103), can be stated as:

- Control what you can, and randomize what you can not.

Randomization, as defined by Hacking (1988, p.428), is

> *"(the) notion of random assignment of treatment to a subset of the plots or persons, leaving the rest as controls. ... I shall speak of an experiment using randomization in this way as involving a randomized design. ...*
> *... There is a related but distinguishable idea of (random) representative sampling."*

As it is usual in the statistical literature, Hacking distinguishes between two intended uses of randomization, namely random design and random sampling. Random design aims to eliminate bias coming from systematic design problems, including several forms of uncontrolled influence, either conscious or unconscious, received from and exerted by agents participating in the experiment. Random sampling, on the other hand, is intended to justify, somehow, assumptions concerning the functional form of a distribution in the statistical model of the experiment. The distinction between random design and random sampling will be kept here, even though, as briefly mentioned in section 6, a deeper probabilistic analysis of randomization shows that, from a theoretical point of view, the two concepts can greatly overlap.

Our immediate interest in randomization (and control) is on whether it can assist the design of experiments by inducing independence relations. This strategy is pinpointed in the following quote from Pearl (2000, p. 340,348. Epilogue: The Art and Science of Cause and Effect):

> *"...Fisher's 'randomized experiment'... consists of two parts, 'randomization' and intervention'."*

> *"Intervention means that we change the natural behavior of the individual: we separate subjects into two groups, called treatment and control, and we convince the subjects to obey the experimental policy. We assign treatment to some patients who, under normal circumstances, will not seek treatment, and give placebo to patients who otherwise would receive treatment. That, in our new vocabulary, means 'surgery' - we are severing one functional link and replacing it with another. Fisher's great insight was that connecting the new link to a random coin flip 'guarantees' that the link we wish to break is actually broken. The reason is that a random coin is assumed to be unaffected by anything we can measure on macroscopic level..."*

3.5   C.S.Peirce and Randomization

We believe that many fine points about the role of randomization in the DSEs can be better understood by following its development from an historical perspective. This is the topic of this section.

In the period of 1850 to 1880 the quantitative analysis of human sensation in response to physical (tactile, acoustic or visual) stimuli, was the main goal of 'psychophysics'. A typical hypothesis in this research program was Fechner's law, see Hernstein and Boring (1966, p.72), which stated that,

> *"The magnitude of sensation (γ) is not proportional to the absolute value of the stimulus (β), but rather to the logarithm of the magnitude of the stimulus when this is expresses in terms of its threshold value (b), i.e. that magnitude considered as unit at which the sensation begins and disappears."*

In modern mathematical notation, $\gamma = k \log(\beta/b) \, I(\beta > b)$.

In his psychophysical experiments Fechner tested his own ability to distinguish the strongest in a pair of stimuli. For example, he would prepare two objects of masses μ and $\mu + \delta$, and later on he would lift them, and 'answer' which one appeared to him to be the heaviest. A quantitative analysis would latter relate the proportion of right and wrong answers with the values of μ and δ, see Stigler (1986, ch.7, Psychophysics as a Counterpoint, p.239-261). Fechner was well aware of the potential difficulties resulting from the fact that the experiments where not performed blindly, that is, since he prepared the experiment himself, he could know in advance the right answer. Nevertheless, he claimed to be able to control himself, be objective, and overcome this difficulty.

According to Dehue (1997), in the decade of 1870, G.E.Müller and several researchers at Tübingen and Göttingen Universities, began to improve the design of psychophysical experiments. The first major improvement was blinding: the stimuli were prepared or administered by an 'Experimenter' or 'Operator' and applied to a distinct person, the 'Observer', 'Patient' or 'Subject', who was kept unaware of the actual intensity of the stimuli.

The second major improvement was the precaution of presenting the stimuli in 'irregular order' (buntem Wechsel). This irregularity was introduced to prevent the patient from becoming habituated to patterns in the sequence of stimuli presented to him or, in other words, to keep him to form building expectations and guessing the right answers. Nevertheless, there was, at that time, neither a general theory defining 'irregularity', nor a systematic method for providing an 'irregular order'.

In 1885, Charles Saunders Peirce and his student Joseph Jastrow presented randomization as a practical solution, in this context, to the question of irregularity, that is,

systematic randomization should prevent any effective guessing by the patient, see Hacking (1988, III. Psychophysics: Peirce's at Work, p.431-434). Peirce was in fact insisting on 'exchangeability', a key notion in the analysis of randomization in modern statistics and, most specially, in Bayesian statistics, that will be discussed in the next section.

Peirce also struggled with the dilemma of allowing or not, in the course of the experiment, sequences that do not 'appear' to be random. His conclusions, see Peirce and Jastrow (1884, p.122), are, once more, precursors to De Finetti's concept of exchangeability:

> *"The pack (of playing-cards) was well shuffled, and, the operator and subject having taken their places, the operator was governed by the color of the successive cards ...*
>
> *A slight disadvantage in this mode of proceeding arises from the long runs of one particular kind of change, which would occasionally be produced by chance and would tend to confuse the mind of the subject. But it seems clear that this disadvantage was less than that which would have been occasioned by his knowing that there would be no such long runs if any means had been taken to prevent them."*

Regardless of its importance, Peirce's solution of randomization was not accepted by his contemporaries, fell into oblivion, and was almost forgotten, until it reappeared much latter in the work of R.A.Fisher. We believe that there are several entangled reasons to explain such a twisted historical process. The psychopysics community raised objections against some of the hypotheses, and also against some methodological aspects presented in Peirce's paper. Besides, there is also a confounding factor generated by a second role played by randomization in Peirce's paper, namely, 'randomization to measure faint effects'. We shall briefly discuss these aspects in the next paragraphs.

Fechner assumed the existence of a threshold (Schwelle), b, bellow which small differences could no longer be discerned. Peirce wanted to refute the existence of this threshold assuming, instead, a continuously decreasing sensitivity to smaller and smaller differences. We should remark that for Peirce this should not have been a fortuitous hypothesis, since it can be related to his general philosophical ideas, most specially with the concept of synechism, see chapter 2, Hartshorne et al. (1992) and Eisele (1976).

Peirce postulated that the patients' sensitivity could be adequately measured by the probability of correct answers, even when the difference was too faint to be consciously discerned by the same patients. Hence, in experiments similar to Fechner's, Peirce asked the patient always to guess the correct answer. Peirce also asked the patient to give the answer a confidence score from 0 to 3. Peirce analyzed his experimental data and derived empirical formulae relating the (rounded) 'subjective' confidence scores, m, and the 'objective' probability of correct answers, p, as in Peirce and Jastrow (1884, p.122):

> " *The average marks seem to conform to the formula* $m = c \log(p/(1-p))$, *where m denotes the degree of confidence on the scale, p denotes the probability of the answer being right, and c is a constant which may be called the index of confidence.*"

At the time of Peirce's experiments, the psychophysical community gave great importance to the analysis of the patient's subjective 'introspections'. According to this view, Peirce's experiments were criticized by asking the patient to guess the correct answer even when he expressed low confidence. Of course, if one understands Peirce's research program, it is clear that that the experimental design he used is perfectly coherent. Unfortunately, this was not the judgment of his contemporaries.

The same techniques and experimental designs used by Peirce were subsequently used by several researchers in attempts to measure faint effects, including effects produced by 'below the consciousness threshold', sub-conscious, or sub-liminal stimuli. Some of these studies were really misconceived, and that may have been yet another contributing factor for the reactions against the use of randomization. Whatever the explanation might be, Peirce's paper fell into oblivion, and the progress of DSEs was delayed by half a century.

3.6   Bayesian Analysis of Randomization

The work of Ronald Aylmer Fisher can undoubtedly be held responsible for disseminating the modern approach to DSEs, including randomization, to almost any area of empirical research, see for example Fisher (1926, 1935). The idea of randomization, however, was later contested by some members of the Bayesian school. Commenting on the use of randomization after Fisher, Hacking (1988, p.429-430), states:

> "*Undoubtedly Fisher won the day, at least for the following generation, but then a new, although not completely unrelated, challenge to randomized design arose. This came from the revival of the 'Bayesian' school, typically associated with L.J.Savage's theory of what he called personal probability. Here the object is to form an initial assessment of one's personal beliefs about a subject and to modify them in the light of experience and a theoretical analysis formally modeled by the calculus of probability and a theory of personal utility. It is widely held to be an almost immediate consequence of this approach that randomization is of no value at all (except perhaps to eliminate some kind of fraud).*"

This erroneous notion of incompatibility between the use of randomization and Bayesian statistics in now completely outdated. One of the most prestigious textbooks in contemporary Bayesian statistics, see Gelman et al. (2003, ch.7, p.198), states:

> *"A naive student of Bayesian inference might claim that because all inference is conditional on the observed data, it makes no difference how those data were collected. This misplaced appeal to the likelihood principle would assert that given (1) a fixed model (including the prior distribution) for the underlying data and (2) fixed observed values of the data, Bayesian inference is determined regardless of the design for the collection of the data. Under this view there would be no formal role for randomization in either sample surveys or experiments. The essential flaw in the argument is that a complete definition of 'the observed data' should include information on how the observed values arose, and in many situations such information has a direct bearing on how these values should be interpreted. Formally then, the data analyst needs to incorporate the information describing the data collection process in the probability model used for analysis."*

Indeed, the classical argument using the likelihood principle against randomization in the DSEs, assumes a fixed, given statistical model and, as concisely stated by Kempthorne (1977, p.16):

> *"The assertion that one does not need randomization in the context of the assumed (linear) model (above) is an empty one because an intrinsic role of randomization is to 'insure' against model inadequacies."*

Gelman et al. (2003, ch.7, p.223-225) proceeds offering a much deeper analysis of the role of randomization from a Bayesian perspective, see also Rubin (1978). The key concept of "ignorable design" specifies decoupling conditions between the sampling (or censoring) process, described by an indicator variable, I, and the distribution of the observed variables, y_{obs}. If the experiment has an ignorable design, we can build a statistical model that explicitly considers y_{obs} alone. Finally, it is ironic that perhaps one of the best arguments for incorporating randomization in Bayesian experimental design is a consequence of de Finetti theorem for exchangeability. As mentioned in section 4, this argument also blurres the distinction between the concepts of randomized design and randomized sampling. We quote, once again, from Gelman et al. (2003, ch.7, p.223-225):

> *"How does randomization fit into this picture? First, consider the situation with no fully observed covariates x, in which case the 'only' way to have an invariant to permutation design - is to randomize."*

> *"In this sense, there is a benefit to using different patterns of treatment assignment for different experiments; if nothing else about the experiments is specified, they are exchangeable, and the global treatment assignment is necessarily randomized over the set of experiments."*

3.7   Randomization, Epistemic Considerations

Several researchers currently concerned with epistemological questions in Bayesian statistics are engaged in a reductionist program dedicated to translate every statistical test or inference problem into a decision theoretic procedure. One of the main proponents and early contributors to this program, but one who also had a much broader perspective, clearly articulating his epistemological insights and motivations, was Bruno de Finetti.

In statistical models our knowledge of the world is encoded in probability distributions. Hence, it is vital to clarify the epistemological or ontological status of probability. Let us examine de Finetti's position, based on his own words, beginning with Finetti (1972, p.189) and Finetti (1980, p.212):

> *"Any assertion concerning probabilities of events is merely the expression of somebody's opinion and not itself an event. There is no meaning, therefore, in asking whether such an assertion is true or false, or more or less probable."*

> *"Each individual making a 'coherent' evaluation of probability (in the sense I shall define later) and desiring it to be 'objectively exact', does not hurt anyone: everyone will agree that this is his subjective evaluation and his 'objectivist' statement will be a harmless boast in the eyes of the subjectivist, while it will be judged as true or false by the objectivist who agree with it or who, on the other hand, had a different one. This is a general fact, which is obvious but insignificant: 'Each in his own way.'   "*

Solipsism, from the Latin solus (alone) +ipse (self), can be defined as the epistemological thesis that the individual's subjective states of mind are the only proper or possible basis of knowledge. Metaphysical solipsism goes even further, stating that nothing really 'exists' outside of one's own mind. From the two above quotations, it is clear that de Finetti stands, if not from a metaphysical, at least from a epistemological perspective, as a true solipsist. This goes farther than many theorists of the Bayesian subjectivist school would venture, but de Finetti charges ahead, with a program that is not only anti-realist, but also anti-idealist. In (1974, V1, Sec.1.11, p.21,22, The Tyranny of Language), de Finetti launches a full-fledged attack against the vain and futile desire for any objective knowledge:

> *"Much more serious is the reluctance to abandon the inveterate tendency of the savages to objectivize and mythologize everything (1); a tendency that, unfortunately, has been, and is, favored by many more philosophers than have struggled to free us from it (2).*

> *(1) The main responsibility for the objectivizationistic fetters inflicted on thought by everyday language rests with the verb 'to be' or 'to exist', and this is why we*

drew attention to it in the exemplifying sentences. From it derives the swarm of pseudoproblems from 'to be or not to be', to 'cogito ergo sum', from the existence of 'cosmic ether' to that of 'philosophical dogmas'.

(2) This is what distinguishes acute minds, who enlivened thought and stimulated its progress, from narrow-minded spirits who mortified and tried to mummify it ... 'great thinkers' (like Socrates and Hume) and 'school philosophers' (like Plato and Kant).

De Finetti was also aware of the dangers of 'objective contamination', that is, any 'objective' (probabilistic) statement can potentially 'infect' and spread its objectivity to other statements, see De Finetti (1974, V2, Sec.7.5.7, p.41-42, Explanations based on 'homogeneity'):

"There is no way, however, in which the individual can avoid the burden of his own evaluations. The key can not be found that will unlock the enchanted garden wherein, among the fairy-rings and the shrubs of magic wands, beneath the trees laden with monads and noumena, blossom forth the flowers of 'Probabilitas realis'. With the fabulous blooms safely in our button-holes we would be spared the necessity of forming opinions, and the heavy loads we bear upon our necks would be rendered superfluous once and for all."

As we have seen in the last sections, a randomization device is built so to provide legitimate 'objective' probabilistic statements about some events, and randomization procedures in DSEs are conceived exactly in order to spread this objectivity around.

I.J.Good was an other leading figure of the early days of the Bayesian revival movement. Contrary to de Finetti, Good has always been aware of the dangers of an extreme subjectivist position, see for example Good (1983, Ch.8 Random Thoughts about Randomness, p.93):

" Some of you might have expected me, as a confirmed Bayesian, to restrict the meaning of the word 'probability' to subjective (personal) probability. That I have not done so is because I tend to believe that physical probability exists and is in any case a useful concept. I think physical probability can be measured only with the help of subjective probability, whereas de Finetti believes that it can be 'defined' in terms of subjective probability. De Finetti showed that if a person has a consistent set of subjective or logical probabilities, then he will behave 'as if' there were physical probabilities, where the physical probability has an initial subjective probability distribution. It seems to me that, if we are going to act if the physical probability exists, then we don't lose anything practical if we assume it really 'does' exist. In fact I am not sure that existence means

more than there are no conceivable circumstances in which the assumption of existence would be misleading. But this is perhaps too glib a definition. The philosophical impact of de Finetti's theorem is that it supports the view that solipsism cannot be logically disproved. Perhaps it is the mathematical theorem with most potential philosophical impact."

In our terminology we would have used the expression 'objective probability' instead of Good's expression, 'physical probability'. In 1962 Good edited a collection of speculative essays, including some on the foundations of statistics. The following short essay by Christopher S.O'D.Scott offers an almost direct answer to de Finetti, see Good (1962, sec.114, p.364-365):

"Scientific Inference: You are given a large number of identical inscrutable boxes. You are to select one, the 'target box', by any means you wish which does not involve opening any boxes, and you then have to say something about is in it. You may do this by any means you wish which does not involve opening the target box.

This apparent miracle can easily be performed. You only have to select the target box at random, and then open a random sample of other boxes. The contents of the sample boxes enable you to make an estimate of the contents of the target box which will be better than a chance guess. To take an extreme case, if none of the sample boxes contains a rabbit and your sample is large, you can state with considerable confidence: 'The target box does not contain a rabbit.' In saying this, you make no assumption whatever about the principles which may have been used in filling the boxes.

This process epitomizes scientific induction at its simplest, which is the basis of all scientific inference. It depends only on the existence of a method of randomization that is, on the assumption that events can be found which are unrelated (or almost) to given events.

It is usually thought that scientific inference depends upon nature being orderly. The above shows that a seemingly weaker condition will suffice: Scientific inference depends upon our knowing ways in which nature is disorderly."

In the preceding chapters we discussed general conditions validating objective knowledge, from a constructivist epistemological perspective. In this chapter we discuss the use of randomization devices, that can generate observable events with distribution that are independent of the distribution of any event relevant to a given statistical study. For example, the statistical study could be concerned with the reaction of human patients affected by a given disease to alternative medical treatments, whereas a "good" randomization device could be a generic 'coin flipping machine', like a regular dice or a mechanical

roulette borrowed from a casino. The randomization device could also be a sophisticated apparatus detecting flips (state transitions) in some quantum system, with transitions probabilities known with a relative precision of one over a trillion.

So far in this chapter we have seen how well can decoupling strategies used in the DSEs, including randomization procedures, help us to perform robust statistical inference and, in doing so, escape, from a pragmatic perspective, the solipsist burdens of an extreme subjectivist position. The same techniques can induce no association relations, generating sparse or structured statistical models. No association hypotheses can then be tested, confirming (or not) such sparse or structured patterns in the statistical model.

3.8   Final Remarks

As analyzed in this chapter, the randomization method, introduced by C.S.Peirce and J.Jastrow (1884), is the fundamental decoupling technique used in the design of statistical experiments (DSEs). Nevertheless, only after the work of R.A.Fisher (1935), were randomized designs used regularly in practice. Today, randomization is one of the basic backbones of statistical theory and methods. Meanwhile, the pioneering work of Peirce had been virtually forgotten by the Statistics community, until rediscovered by the historical research of Stigler (1978) and Hacking (1988). Nevertheless, even today, the work of Peirce is presented as an isolated and ad hoc contribution. As briefly indicated in section 5, it is plausible that Peirce and Jastrow's experimental and methodological work could have had motivations related to more general ideas of Peircean philosophy. In particular, we believe that the faint effects psychophysical hypothesis can be liked to the concept of synechism, while the randomized design solution can be embedded in the epistemological framework of Peirce's objective idealism. We believe that these topics deserve the attention of further research.

In this chapter we have examined some aspects of DSEs, such as blocking, control and randomization, from an epistemological perspective. However, in many applications, most noticeably in medical studies, several other aspects have to be taken into account, including the well being of the patients taking part in the study. In our view, such complex situations require a thorough, open and honest discussion of all the moral and ethical aspects involved. Typically they also demand sound protocols and complex statistical models, suited to the fine quantitative analyses needed to balance multiple objectives and competing goals. For the Placebo, Nocebo, Kluge Hans, and similar effects, and the importance of blinding and randomization in clinical trials, see Kotz et al. (2005), under the entries Clinical Trials I, by N.E.Breslow, v.2, p.981-989, and Clinical Trials II, by R.Simon, v.2, p.989-998. For additional references on statistical randomization procedures, see Folks (1984), Kadane and Seidenfeld (1990), Kaptchuk and Kerr (2004), Karlowski et al. (1975), Kempthorne (1977, 1980), Noseworthy et al. (1994), Pfeffermann

et al. (1998) and Skinner and Chambers (2003).

Chapter 4

Metaphor and Metaphysics: The Subjective Side of Science

"Why? - That is what my name asks!
And there He blessed him."
Genesis, XXXII, 30.

"Metaphor is perhaps one of man's most fruitful potecialities.
Its efficacy verges on magic, and it seems a tool for creation
which God forgot inside His creatures when He made them."
José Ortega y Gasset, The Dehumanization of Art, 1925.

"There is nothing as practical as a good theory."
Attrituted to Ludwig Boltzmann (1844-1906).

4.1   Introduction

In this chapter we proceed with the exploration of the Cognitive Constructivism epistemological framework (Cog-Con), continuing the previous work developed in previous chapters, and briefly reviewed in section 5. In the previous chapters, we analyzed questions concerning *How* objects (eigen-solutions) emerge, that is, How they (eigen-solutions) become known in the interaction processes of a system with its environment. These questions had to do with laws, patterns, etc., expressed as sharp or precise hypotheses, and we argued that statistical hypothesis testing plays an important role in their validation.

It is then natural to ask - *Why?* Why do these objects are (the way they are) and interact the way they do? Why-questions claim for a causal nexus in a chain of events.

Therefore, their answers must be theoretical constructs based on interpretations of the laws used to describe these events. This chapter is devoted to the investigation of these issues. Likewise, the interplay between the How and Why levels of inquiry which, in the constructivist perspective, are not neatly stratified in separate hierarchical layers, but interact in complex (often circular) patterns, will also be analyzed. As in the previous chapters, the discussion is illustrated by concrete mathematical models. In the process, we raise some interesting questions related to the practice of statistical modeling.

Sections 2 examines the dictum "Statistics is Prediction". The importance of accurate prediction is obvious for any statistics practitioner, but is that all there is? The investigation on the importance of model interpretability begins in section 3, the rhetorical power of mathematical models, self-fulfilling prophecies and some related issues are discussed and a practical consulting case in Finance, concerning the detection of trading opportunities for intraday operations in both the *BOVESPA* and *BM&F* financial markets is presented. In this example, the REAL classification tree algorithm, a statistical technique presented in Lauretto et al. (1998), is used.

Section 4 is devoted to the issue of language dependence. Therein, the investigation on model interpretability continues with an analysis of the eternal counterpointing issues of models for prediction and models for insight. An example from Psychology, concerning dimensional personality models is also presented. These models are based on a dimension reduction technique known as Factor Analysis.

In section 6, the necessary or "only world" vs. optimal or "best world" formulations of optics and mechanics are discussed. Simple examples related to the calculus of variations, are presented, which abridge the epistemological discussion in the following sections. Section 7 discusses efficient and final causal relations, teleological explanations, necessary and best world arguments, and the possibility or desirability of having multiple interpretations for the same model or multiple models for the same phenomenon. In section 8, the form of modern metaphysical arguments in the construction of physical theories is addressed.

In section 9, some simple but widely applicable models based on averages computed over all "possible worlds", or more specifically, path integrals over all possible trajectories of a system, are presented. The first example in this section relates to the linear system Monte Carlo solution to the Dirichlet problem, a technique driven by a stochastic process known as Gaussian Random Walk or Brownian Motion. Section 9 also points out to a generalization of this process known as Fractional Brownian Motion. In sections 7 to 9 we also try to examine the interrelations between "only world", "best world" and "possible worlds" forms of explanation, as well as their role and purpose in the light of cognitive constructivism, since they are at the core of modern metaphysics.

Section 10 discusses how hypothetical models, mathematical equations, etc., relate to the "true nature" of "real objects". The importance of this relationship in the history of science is illustrated therein with two cases: The Galileo affair, and the atomic or

molecular hypothesis, as presented by L.Boltzmann, A.Einstein and J.Perrin. In section 11 our final remarks are presented.

All discussions in the paper are motivated with illustrative examples, and these examples follow an approximate order from soft to hard science. The example of Psychology presented at section 4, together with the corresponding Factor Analysis modeling technique, is at an intermediate point of this soft-hard scale, making it a natural place for making a pause, taking a deep breath, and trying to get a bird's eye view of the panorama. Section 5 reviews some concepts of Cog-Con ontology defined in previous chapters, and discusses some insights on Cog-Con metaphysics.

4.2   Statistics is Prediction. Is that all there is?

As a first example for discussion, we present a consulting case in finance. The goal of this project was to implement a model for the detection of trading opportunities for intraday operations in both the *BOVESPA* and the *BM&F* financial markets. For details we refer to Lauretto et al. (1998). The first algorithms implemented were based on Polynomial Networks, as presented in Farlow (1984) and Madala and Ivakhnenko (1994), combined with standard time series pre-processing analysis techniques such as de-trending, de-seasonalization, differencing, stabilization and linear transformation, as exposed in Box and Jenkins (1976) and Brockwell and Davis (1991). A similar model is presented in Lauretto et al. (2009). The predictive power of the Polynomial Network model was considered good enough to render a profitable return / risk performance.

According to the decision theoretic theory, and its gambling metaphor as presented in section 1.5, the fundamental purpose of a statistical model is to help the user in a specific gambling operation, or decision problem. Hence, at least according to the orthodox Bayesian view, predictive power is the basic criterion to judge the quality of a statistical model. This conclusion is accepted with no reservations by most experts in decision theory, orthodox Bayesian epistemologists, and even by many general practitioners. As typical examples, consider the following statements:

"We assume that the primary aim of [statistical] analysis is prediction." Robert (1995, p.456).

"Although association with theory is reassuring, it does not mean that a statistical fitted model is more true or more useful. All models should stand or fall based on their predictive power." Newman and Strojan (1998, p.168).

"The only useful function of a statistician is to make predictions, and thus to provide a basis for action." W.E.Demming, as quoted in W.A.Wallis (1980).

"It is my contention that the ultimate aim of any statistical analysis is to forecast, and that this determines which techniques apply in particular cir-

> *cumstances... The idea that statistics is all about making forecasts based on probabilistic models of 'reality' provides a unified approach to the subject. In the literary sense, it provides a consistent authorial 'voice'... the underlying purpose, often implicit rather than explicit, of every statistical analysis is to forecast future values of a variable.*" A.L.McLean (1998).

Few theaters of operation so closely resemble a real casino as the stock market, hence, we were convinced that our model would be a success. Unfortunately, our Polynomial Network model was not well accepted by the client, that is, it was seldomly used for actual trading. The main complaint was the model's lack of interpretability. The model was perceived as cryptic, a "black box" capable of selecting strategic operations and computing predicted margins and success rates, but incapable of providing an explanation of *Why* the selection was recommended in the particular juncture. This state of affairs was quite frustrating indeed: First, the client had never explicitly required such functionality during the specification stage of the project, hence the model was not conceived to provide explanatory statements. Second, as a fresh Ph.D. in Operations Research, I was well trained in the minutiae of Measure Theory and Hilbert Spaces, but had very little experience on how to make a model that could be easily interpreted by somebody else. Nevertheless, since (good) costumers are always right, a second model was specified, developed and implemented, as explained in the next section.

4.3   Rhetoric and Self-Fulfilling Prophecies

The first step to develop a new model for the problem presented in the last section, was to find out what the client meant by an interpretable model. After a few brainstorm sessions with the client, we narrowed it down to two main conditions: understandable I/O and understandable rules. The first condition (understandable I/O) called for the model's input and output data to be already known, familiar or directly interpretable. The second condition (understandable rules) called for the model's transformation functions, re-presentation maps or derivation rules to be also based in already known, familiar or directly interpretable principles.

Technical Indicators, derived from pre-processed price and volume trading data, constituted the input to the second model. Further details on their nature will be given later in this section. For now, it is enough to know that they are widely used in financial markets, and that the client possessed ample expertise in technical analysis. The model's statistical data processing, on the other hand, was based on a classification tree algorithm specially developed for the application - the Real Attribute Learning Algorithm, or REAL, as presented in Lauretto et al. (1998). For general classification tree algorithms, we refer to Breiman (1993), Denison et al. (2002), Michie et al. (1994), Mueller and Wysotzki (1994), and Unger and Wysotzki (1981).

The REAL based model turned out to be very successful. In fact, statistically, it performed almost as well as the Polynomial Network model, under the performance metric specified in Lauretto et al. (1998). Moreover, when combined with a final interpretive analysis and go-ahead decision from the traders, the REAL based model performed better than the Polynomial Network model. The model was finally put into actual use, once it was perceived as interpretable and understandable. Since a large part of our consulting fees depended on the results in actual trading, this was an important condition for getting fair economical compensation for all this intellectual endeavor.

As already mentioned, we were intrigued at the time (and still are) by many aspects related to model interpretation and understanding. In this section we begin to analyse this and other similar issues. Concerning first the very need for explanations: Humans seem to be always avid for explanations. They need them in order to carry out their deeds, and they want them to be based on already known schemata, as acknowledged in Damodaran (2003,ch.7,p.17):

> *"The Need for Anchors: When confronted with decisions, it is human nature to begin with the familiar and use it to make judgments. ...*
>
> *The Power of the Story: For better or worse, human actions tend to be based not on quantitative factors but on story telling. People tend to look for simple reasons for their decisions, and will often base their decision on whether these reasons exist."*

The rhetorical purpose and power of statistical models have been able to conquer, within the statistical literature, only a small fraction of its relative importance in the consulting practice. There are, nevertheless, some remarkable exceptions, as see for example, in Abelson (1995, p.xiii):

> *"The purpose of statistics is to organize a useful argument from quantitative evidence, using a form of principled rhetoric. The word* principled *is crucial. Just because rhetoric is unavoidable, indeed acceptable, in statistical presentations does not mean that you should say anything you please."*
>
> *"Beyond the rhetorical function, statistical analysis also has a narrative role. Meaningful research tells a story with some point to it, and statistics can sharpen the story."*

Let us now turn our attention to the inputs to the REAL based model, the Technical Indicators, also known as Charting Patterns. For a general description, see Damodaran (2003,ch.7). For some of the indicators used in the REAL project, see Colby (1988) and Murphy (1986). Technical indicators are primarily interpreted as behavioral patterns in the markets or, more appropriately, as behavioral patterns of the market players. Damodaran defines five groups that categorize the indicators according to the dominant

aspects of the behavioral pattern. A concise description of these five groups of indicators is given in Damodaran (2003,ch.7,p.46-47):

> 1 - External Forces / Large Scale Indicators: *"If you believe that there are long-term cycles in stock prices, your investment strategy may be driven by the cycle you subscribe to and where you believe you are in the cycle."*
> 2 - Lead / Follow Indicators: *"If you believe that there are some traders who trade ahead of the market, either because they have better analysis tools or information, your indicators will follow these traders - specialist short sales and insider buying/selling, for instance - with the objective of piggy-backing on their trades."*
> 3 - Persistence / Momentum Indicators: *"With momentum indicators, such as relative strength and trend lines, you are assuming that markets often learn slowly and that it takes time for prices to adjust to true values."*
> 4 - Contrarian / Over Reaction Indicators: *"Contrarian indicators such as mutual fund holdings or odd lot ratios, where you track what investors are buying and selling with the intention of doing the opposite, are grounded in the belief that markets over react."*
> 5- Change of Mind / Price-Value Volatility Indicators: *"A number of technical indicators are built on the presumption that investors often change their views collectively, causing shifts in demand and prices, and that patterns in charts - support and resistance lines, price relative to a moving average- can predict these changes."*

At this point, it is important to emphasize the dual nature of technical indicators: They disclose some things that may be happening with the trading market and also some things that may be happening with the traders themselves. In other words, they portray dynamical patterns of the market that reflect behavioral patterns of the traders.

Two characteristics of the REAL based model, of vital importance to the success in the consulting case presented, relate to rhetorical and psychological aspects that have been commented so far:

- Its good predictive and rhetorical power, which motivated the client to trade on the basis of the analyses provide by the model;

- The possibility of combining and integrating the analyses provided by the model with expert opinion.

Technical indicators often carry the blame of being based in self-fulfilling prophecies, over-simplified formulas, superficial and naive behavioral patterns, unsound economic grounds, etc. From a pragmatic perspective, market analysts do not usually care about technical analysis compatibility with sound economic theories, mathematical sophistication, etc. Its ability to detect trading opportunities is what counts. From a conceptual

perspective, each of these analyses does tell a story about a cyclic reinforcement or correction (positive or negative feed-back) mechanism in the financial system. What is peculiar about self-fulfilling prophecies is that the collective story telling activity is a vital link in the feed-back mechanism. It is not surprising then that the market players' perception of how good the story itself looks should play an important role in fortelling whether the prophecy will come true. From this perspective one can understand the statement in Murphy (1986, p.19):

> *"The self-fulfilling prophecy (argument) is generally listed as a criticism of charting. It might be more appropriate to label it as a compliment."*

The importance of the psychological aspects of the models studied in this section motivate us to take a look, in the sequel, at some psychological models of personality.

4.4 Language, Metaphor and Insight

In chapter 1, the dual role played by Statistics in scientific research, namely, predicting experimental events and testing hypotheses, was pointed out. It was also emphasized that, under a constructivist perspective, these hypotheses are often expressed as equations of a mathematical model. In the last section we began to investigate the importance of the interpretability of these models. The main goal of this section is to further investigate subjective aspects of a statistical or mathematical model, specifically, the understanding or *insight* it provides.

We start with three diffent versions of the well-known motto of Richard Hamming:

- *"The purpose of models is insight, not numbers."*

- *"The purpose of computing is insight, not numbers."*

- *"The purpose of numbers is insight, not numbers."*

Dictionary definitions of Insight include:

- A penetrating, deep or clear perception of a complex situation;

- Grasping the inner or hidden nature of things;

- An intuitive or sudden understanding.

The illustrative case presented in this section is based on psychological models of personality. Many of these models rely on symmetric configurations known as "mandala" schemata, see for example Jung (1968), and a good example is provided by the five elements model of traditional Chinese alchemy and their associated personality traits:

1- Fire: Extroverted, emotional, emphatic, self-aware, sociable, eloquent.

2- Earth: Caring, supporting, stable, protective, worried, attached.

3- Metal: Analytical, controlling, logical, meticulous, precise, zealous.

4- Water: Anxious, deep, insecure, introspective, honest, nervous.

5- Wood: Angry, assertive, creative, decisive, frustrated, leading.

Interactions between elements are conceived as a double feed-back cycle, represented by a pentagram inscribed in a pentagon. The pentagon or external cycle represent the creation, stimulus or positive feed-back in the system, while the pentagram or internal cycle represent the destruction, control or negative feed-back in the system. The traditional representation of these systemic generative mechanisms or causal relations are:

Pentagon: fire $[calcinates\ to\ \rangle$ earth $[harbors\rangle$ metal $[condenses\rangle$ water $[nourishes\rangle$ wood $[fuels\rangle$ fire.

Pentagram: fire $[melts\rangle$ metal $[cuts\rangle$ wood $[incorporates\rangle$ earth $[absorbs\rangle$ water $[extinguishes\rangle$ fire.

This double feed-back structure allows the representation of system with complex interconnections and nontrivial dynamical properties. In fact, the systemic interconnections are considered the key for understanding a general five-element model, rather than any superficial analogy with the five elements' traditional labels.

It is an entertaining exercise to compare and relate the five alchemical elements listed above with the five groups of technical indicators presented in the last section, or with the big-five personality factors presented next, even if some of these models are considered pre-scientific. Why, for example, do these models employ exactly five factors? That is, why is it that "four are few and six are many"? Is there an implicit mechanism in the model, see Hargittai (1992), Hotchkiss (1998) or Philips (1995, ch.2), or is this an empirical statement supported by research data?

Scientific psychometric models must be based on solid statistical analysis of testable hypotheses. Factor Analysis has been one of the preferred techniques used in the construction of modern psychometric models and it is the one used in the examples we discuss next. In section C.5, the basic structure of factor analysis statistical models is reviewed.

In Allport and Odbert (1936) the authors presented their Lexical Hypothesis. According to them, important aspects of human life correspond to words in the spoken language. Also the number of corresponding terms in the lexicon is supposed to reflect the importance of each aspect:

"Those individual differences that are most salient and socially relevant in peoples lives will eventually become encoded into their language; the more important such a difference, the more likely is it to become expressed as a single word."

One of the most widely used factor model takes into account five factors or personality traits. These are the five dimensions of the "OCEAN" personality model or "big-five". Further details on the meaning of these factors can be found in Shelder and Westen (2004), from the list of the most relevant factor loadings. The "OCEAN" labels, ordered according to their statistical relevance, are:

1- Extraversion, Energy, Enthusiasm;

2- Agreeableness, Altruism, Affection;

3- Conscientiousness, Control, Constraint;

4- Neuroticism, Negative Affectivity, Nervousness;

5- Openness, Originality, Open-mindedness.

Subsequent studies pointed to the "existence" of more factors, for a review of several of such models, see Widiger and Simonsen (2005). Herein, we focus our attention in the 12-factor model of Shelder and Westen. We remark, however, that the publication of the 12-factor model, fired an inflamed literary debate concerning the necessity (or not) of more than 5 factors. In the quotation below, Shelder and Westen (2004, p.1752-1753) pinpoint the issue of language dependence in the description of reality, an issue of paramount importance in cognitive constructivism and one of the main topics analyzed in this section.

> *"Applying the Lexical Hypothesis to Personality Disorders:*
>
> *Ultimately, the five-factor model is a model of personality derived from the constructs and observations of lay-people, and it provides an excellent map of the domains of personality to which the average layperson attends. However, the present findings suggest that the five-factor model is not sufficiently comprehensive for describing personality disorders or sophisticated enough for clinical purposes.*
>
> *In contrast to laypeople, practicing clinicians devote their professional lives to understanding the intricacies of personality. They develop intimate knowledge of others lives and inner experience in ways that may not be possible in everyday social interaction. Moreover, they treat patients with variants of personality pathology that laypeople encounter only infrequently (and are likely to avoid when they do encounter it). One would therefore expect expert clinicians to develop constructs more differentiated than those of lay observers.*
>
> *Indeed, if this were not true, it would violate the lexical hypothesis on which the five-factor model rests: that language evolves over time to reflect what is important. To the extent that mental health professionals observe personality with particular goals and expertise, and observe the more pathological end of the personality spectrum, the constructs they consider important should differ from those of the average layperson."*

The issue of language dependence is very important in cognitive constructivism. For further discussion, see Maturana (1988, 1991). Thus far we have stressed the lexical aspect of language, that is, the importance of the available vocabulary in our description of reality. In the remaining part of this section we shall focus on the symbolic or figurative use of the language constructs in these descriptions. We proceed by examining in more detail the factor analysis model.

Factor analysis is a dimension reduction technique. Its application renders a 'simple' object, the factor model, capable of efficiently "coding", into a space of reduced dimension, a complex 'real' object from a full or high dimensional space. In other words, a dimension reduction technique presumes some form of valid knowledge transference, back and forth the complex (high dimensional) object and its simple (low dimensional) model. Hence, the process of using and interpreting factor analysis models can be conceived as metaphorical. Recall that the Greek word metaphor stands for transport or transfer, so that a linguistic metaphor transfers some of the characteristics of one object, called the source or vehicle, into a second distinct object, called the target, tenant or topic; for a comprehensive reference see Lakoff and Johnson (2003).

For reasons which are similar to those studied in the last section, most users of a personality model require it to be statistically sound. Many of them further demand it to be interpretable, in order to provide good insights to their patient's personality and problems. A good model should not only be useful in predicting recovery rates or drug effectiveness, but also help in supplying good counseling or therapeutics.

Paraphrasing Vega-Rodríguez (1998):

The metaphorical mechanism should provide an articulation point between the empirical and the hypothetical, the rational and the intuitive, between calculation and insight.

The main reason for choosing factor analysis to illustrate this section is its capability of efficiently and transparently building sound statistical models that, at the same time, provide intuitive interpretations. While soundness is the result of "estimation and identification tools", such as ML (maximum likelihood) or MAP (maximum a posteriori) optimization, hypothesis testing and model selection, interpretableness results from "representation tools", such as orthogonal and oblique factor rotation techniques.

Factor rotation tools are meant to reconfigure the structure of a given factor analysis model, so as to maintain its probabilistic explanatory power while maximizing its heuristic explanatory power. Factor rotations are performed to implement an objective optimization criteria, such as sparsity or entropy maximization. The optimal solution (for each criterion) is unique and hoped to enhance model interpretability a great deal.

4.5 Constructive Ontology and Metaphysics

How important heuristic arguments are in other areas of science? Should statistical or mathematical models play a similar rhetorical role in other fields of application? We will try to answer these questions by discussing the role played by similar heuristic arguments in physics. In sections 2 and 3 we dealt with application areas in which text(ure) manufacture comprised, to a great extent, the very spinning of the threads. Nevertheless, one can have the false impression that the constructivist approach suits better high level, soft science areas, rather than low level, rock bottom Physics. This widely spread misconception is certainly not the case. In sections 7 through 10 we analyze the role played in science by metaphysics, a very special form of heuristic argumentation.

The example presented in section 4, together with the corresponding Factor Analysis modeling technique, is at an intermediate point of the soft-hard science scale used herein to (approximately) order the examples. Therefore, as previously stated in the introduction, we shall use section the current section to make a pause in the exposition, take a deep breath, and try to get a bird's eye view of the scenario. This section also reviews some concepts of Cog-Con ontology defined in previous chapters and discusses some insights on Cog-Con metaphysics.

The Cog-Con framework rests upon two basic metaphors: the Heinz von Forster's metaphor of *Object as token for an eigensolution*, which is the key to Cog-Con ontology, and the Humberto Maturana and Francisco Varela's metaphor of *Autopoiesis and cognition*, the key to Cog-Con metaphysics. Below we review these two metaphors, as they where used in chapter 1.

Autopoiesis and Cognition

Autopietic systems are non-equilibrium (dissipative) dynamical systems exhibiting (meta) stable structures, whose organization remains invariant over (long periods of) time, despite the frequent substitution of their components. Moreover, these components are produced by the same structures they regenerate. As an example, take the macromolecular population of a single cell, which can be renewed thousands of times during its lifetime, see Bertalanffy (1969). However, in spite of the fact that autopoiesis was a metaphor developed to suit the essential characteristics of organic life, the concept of autopoietic system has been applied in the analysis of many other concrete or abstract autonomous systems such as social systems and corporate organizations, see for example Luhmann (1989) and Zelleny (1980).

The regeneration processes in the autopoietic system production network require the acquisition of resources such as new materials, energy and neg-entropy (order), from the system's environment. Efficient acquisition of the needed resources demands selective

(inter)actions which, in turn, must be based on suitable inferential processes (predictions). Moreover, these inferential processes characterize the agent's domain of interaction as a cognitive domain. For more details see the comments in chapter 1 and, more importantly, the original statements in Maturana and Varela (1980, p.10):

> "The circularity of their organization continuously brings them back to the same internal state (same with respect to the cyclic process). ... Thus the circular organization implies the prediction that an interaction that took place once will take place again. ... Accordingly, the predictions implied in the organization of the living system are not predictions of particular events, but of classes of inter-actions. ... This makes living systems, inferential systems, and their domain of interactions a cognitive domain."

Object as Tokens for Eigen-Solutions

The circular (cyclic or recursive) characteristic of autopoietic regenerative processes and their eigen (auto, equilibrium, fixed, homeostatic, invariant, recurrent, recursive) -states, both in concrete and abstract autopoietic systems, are investigated in Foerster (2003) and Segal (2001).

> "The meaning of recursion is to run through one's own path again. One of its results is that under certain conditions there exist indeed solutions which, when reentered into the formalism, produce again the same solution. These are called "eigen-values", "eigen-functions", "eigen-behaviors", etc., depending on which domain this formation is applied - in the domain of numbers, in functions, in behaviors, etc." Segal (2001, p.145).

The concept of eigen-solution for an autopoietic system is the key to distinguish specific objects in a cognitive domain.

> "Objects are tokens for eigen-behaviors. Tokens stand for something else. In exchange for money (a token itself for gold held by one's government, but unfortunately no longer redeemable), tokens are used to gain admittance to the subway or to play pinball machines. In the cognitive realm, objects are the token names we give to our eigen-behavior. ... When you speak about a ball, you are talking about the experience arising from your recursive sensorimotor behavior when interacting with that something you call a ball. The "ball" as object becomes a token in our experience and language for that behavior which you know how to do when you handle a ball. This is the constructivist's insight into what takes place when we talk about our experience with objects." Segal (2001, p.127).

Furthermore, von Foerster establishes four essential attributes of eigen-solutions:

> "Eigenvalues have been found ontologically to be discrete, stable, separable and composable, while ontogenetically to arise as equilibria that determine themselves through circular processes. Ontologically, Eigenvalues and objects, and likewise, ontogenetically, stable behavior and the manifestation of a subject's "grasp" of an object cannot be distinguished." Foerster (2003, p.266).

Constructive Ontology

The Cog-Con framework also includes the following conception of reality and some related terms, as defined in chapter 2:

> *1. Known (knowable) Object:* An actual (potential) eigen-solution of a given system's interaction with its environment. In the sequel, we may use a somewhat more friendly terminology by simply using the term Object.
>
> *2. Objective (how, less, more):* Degree of conformance of an object to the essential attributes of an eigen-solution (to be precise, stable, separable and composable).
>
> *3. Reality:* A (maximal) set of objects, as recognized by a given system, when interacting with single objects or with compositions of objects in that set.

The Cog-Con framework assumes that an object is always observed by an observer, just like a living organism or a more abstract system, interacting with its environment. Therefore, this framework asserts that the manifestation of the corresponding eigen-solution and the properties of the object are respectively driven and specified by both the system and its environment. More concisely, Cog-Con sustains:

> *4. Idealism:* The belief that a system's knowledge of an object is always dependent on the systems' autopoietic relations.
>
> *5. Realism:* The belief that a system's knowledge of an object is always dependent on the environment's constraints.

Consequently, the Cog-Con perspective requires a fine equilibrium, called *Realistic or Objective Idealism. Solipsism or Skepticism* are symptoms of an epistemological analyses that loose the proper balance by putting too much weight on the idealistic side. Conversely, *Dogmatic Realism* is a symptom of an epistemological analyses that loose the proper balance by putting too much weight on the realistic side. Dogmatic realism has been, from the Cog-Con perspective, a very common (but mistaken) position in modern epistemology. Therefore, it is useful to have a specific expression, namely, *something in*

Experiment   Theory

Operation-alization	$\Leftarrow$ Experiment design	$\Leftarrow$ Hypotheses formulation
$\Downarrow$		$\Uparrow$
Effects observation	True/False eigen-solution	Creative interpretation
$\Downarrow$		$\Uparrow$
Data acquisition	$\Rightarrow$ Mnemetic explanation $\Rightarrow$	Statistical analysis

Sample space   Parameter space

Figure 1: Scientific production diagram.

itself to be used as a marker or label for such ill posed dogmatic statements. The method used to access something in itself is often described as: - Something that an observer would observe if the (same) observer did not exist, or - Something that an observer could observe if he made no observations, or - Something that an observer should observe in the environment without interacting with it (or disturbing it in any way), and many other equally senseless variations.

Although the application of the Cog-Con framework is as general as that of autopoiesis, this paper is focused on scientific activities. The interpretation of scientific knowledge as an eigensolution of a research process is part of a Cog-Con approach to epistemology. Figure 1 presents an idealized structure and dynamics of knowledge production, see Krohn and Küppers (1990) and chapters 1 and 6. The diagram represents, on the Experiment side (left column) the laboratory or field operations of an empirical science, where experiments are designed and built, observable effects are generated and measured, and an experimental data bank is assembled. On the Theory side (right column), the diagram represents the theoretical work of statistical analysis, interpretation and (hopefully) understanding according to accepted patterns. If necessary, new hypotheses (including whole new theories) are formulated, motivating the design of new experiments. Theory and experimentation constitute a double feed-back cycle making it clear that the design of experiments is guided by the existing theory and its interpretation, which, in turn, must be constantly checked, adapted or modified in order to cope with the observed experiments. The whole system constituting an autopoietic unit.

Fact or Fiction?

At this point it is useful to (re)turn our attention to a specific model, namely, factor analysis, as discussed in section 4, and consider the following questions raised by Brian Everitt (1984, p.92, emphases are ours) concerning the appropriate interpretation of factors:

> " **Latent variables - fact or fiction?** One of the major criticisms of factor analysis has been the tendency for investigators to give names to factors, and subsequently, to imply that these factors **have a reality of their own over and above the manifest variables.** This tendency continues with the use of the term latent variables since it suggests that they are existing variables and that there is simply a problem of how they should be measured. In truth, of course, latent variables will never be anything more than is contained in the observed variables and will never be anything beyond what has been specified in the model. For example, in the statement that verbal ability is whatever certain test have in common, the empirical meaning is nothing more than a shorthand for the observations of the correlations. It does not mean that verbal ability is a variable that is measurable in any manifest sense. However, the concept of latent variable may still be extremely helpful. A scientist may have a number of hypothetical constructs in terms of which some theory is formulated, and he is willing to assume that the latent variables used in specifying the structural models of interest are the operational equivalents to theoretical constructs. As long as it is remembered that in most cases there is no empirical way to prove this correspondence, then such an approach can lead to interesting and informative **theoretical insights**."

Ontology is a term used in philosophy in reference to a systematic account of *existence* or *reality*. We have already established the Cog-Con approach to objects as tokens for eigen-solutions, and explained their four essential attributes, namely, discreteness (preciseness, sharpness or exactness), stablity, separability and composability. Therefore, in the Cog-Con framefwork, accessing the ontological status of an object, or to say how objective it is, is to ascertain how well it manifests the four essential attributes of an eigen-solution.

The Full Bayesian Significance Test, or FBST, is a possibilistic belief calculus, based on (posterior) probabilistic measures, that was conceived as a statistical significance test to access the objectivity of an eigen-solution, that is, to measure how well a given object manifests or conforms to von Foerster's four essential attributes. The FBST belief or credal value, $\text{ev}(H \,|\, X)$, the *e-value* of hypothesis H given the observed data X, is interpreted as the *epistemic value* of hypothesis H (given X), or the *evidence value* of data X (supporting H). The formal definition of the FBST and several of its implementation in

specific problems can be found in the author's previous publications, and are reviwed in appendix A.

Greek or Latin? Latent or Manifest?

We have already discussed the ontological status of an object. This discussion assumes testing hypotheses in a statistical model which, in order to built, one must know how to distinguish concrete measurable entities from abstract concepts, observed values from model parameters, latent from manifest variables, etc. When designing and conducting an experiment, a scientist must have a well defined a statistical model, and keep these distinctions crisp and clear. This is so important in the experimental sciences that statisticians have the habit of using Latin letters for observables, and Greek letters for parameters. When a statistician questions whether a letter is Latin or Greek, he or she is not asking for help with foreign alphabets, but rather seeking information about the aforementioned distinctions.

According to the positivist philosophical school, measurable entities, observed values, manifest variables, etc. are the true, first class entities of a hard science, while abstract concepts, model parameters, latent variables, etc. should be considered second class entities. One reason for downgrading the later class is that the positivist school assumes a nominalist perspective. Nominalism (at least in its strictest form) considers abstract concepts as mere names *(nomina)*, that may stand as proxy for a "really existing item", denoting "that singular thing" *(supponere pro illa re singulari)*. The Cog-Con perspective plays no role in the positivist dream. This issue will be further investigated in the next sub-section, as well as in sections 8 and 11. For now we offer the following argument:

Although for a given model, the aforementioned distinctions between what to write using Latin or Greek letters should be always crisp and clear, we may have to simultaneously work with several models. For example, we may need to use several models hierarchically organized to cope with phenomena at different scales or levels of granularity, like models in physics, chemistry, biology, and psychology, see chapters 5 and 6. We may also need different models for competing theories trying to explain a given phenomenon. Finally, we may need different models providing equivalent or compatible laws to given phenomena that, nevertheless, use distinct theoretical approaches, see section 8, 9 and 10. The positivist dream quickly turns into a nightmare when one realizes that an entity corresponding to a Greek letter variable in one model corresponds to a Latin letter variable in another, and vice-versa.

It is also important to realize that in the Cog-Con approach the ontological status of an object is a reference to the properties of the corresponding eigen-solution emerging in a cyclic process. This leads to an intrinsically dynamic approach to ontology, in sharp contrast with other analyses based on static categories. A consequence of this dynamical setting is that in the Cog-Con approach a statement about the ontological status of

a single element or isolated component in a process is an indirect reference to its role in the emergence of the corresponding eigen-solution. Equivalent or similar elements may play very different roles in distinct processes. Such distinct or multiple roles will not pose conceptual difficulties to the Cog-Con framework as long as the corresponding (statistical) models are clearly stated and well defined. For interesting examples of this situation, typical of modular and hierarchical architectures, hypercyclical organization, and emergent properties, see chapters 5 and 6.

Constructive Metaphysics

Metaphysics, in its gnosiological sense, is a philosophical term we use to refer to a systematic account of possible forms of understanding, valid forms of explanation or rational principles of intelligibility. In science, such explanations are often well represented in a schematic diagram describing the organization of a conceptual network. A link in such a diagram expresses a theoretical relation like, for example, a causal nexus, that is, a cause and effect relation. In modern science, such explanations must also include the symbolic derivation of scientific hypotheses from general scientific laws, the formulation of new laws in an existing theory, and even the conception of new theories, as well as their general understanding based on general metaphysical principles.

In this context, it is natural to ask questions like: What do we mean by the intuitive quality or theoretical importance of a concept or, more generally, of a sub-network? How interesting are the insights we gain from it? How can we access its explanatory power or heuristic value? We will try to answer these questions in the following sections, most specially in section 8, on modern metaphysics. In this section we provide only a preliminary discussion of the importance of metaphysical entities in the constructivist perspective.

We now return to Humberto Maturana and Francisco Varela's metaphor of autopoiesis and cognition. As stated at the beginning of this section this metaphor is the key for Cog-Con metaphysics. From details of this metaphor we conclude that the autopoietic relations of a system not only define who or what it "is", but also limit the class of interactions in which it can possibly engage or the class of events it can possibly perceive. An adaptive system can learn, that is, it can reconfigure its internal organization, reshape its architecture, in order to enlarge its scope of inference or make better predictions. Nevertheless, learning is an evolutive process, and any evolutionary path to the future has to progress from the system's present (or initial) configuration. From the above considerations it is clear that, from a constructivist perspective, the specification of autopoietic relations are of vital importance since they literally define the scope and possibilities of the system's life.

Theoretical Insights

Cog-Con approaches science as an autopoietic system whose organization is coded by symbolic laws, causal relations, and metaphysical principles. Consequently, we must give them the greatest importance. Nevertheless, such metaphysical entities are even more abstract than the latent variables discussed in the last subsection. In contrast with the constructivist approach, the positivist school is thus quite hostile to metaphysical concepts.

In the Cog-Con perspective, metaphysics provides meaning to objects in a give reality, explaining *why* the corresponding eigen-solutions manifest themselves the way they do. Accordingly, theoretical concepts become building blocks in the coding of systemic knowledge and reference marks in the mapping of the systems environment. Conceptual relations are translated into inference tools, thus becoming, by definition, the basis of autopoietic cognition. In the Cog-Con perspective, better understanding will strengthen a given theoretical architecture or entail its evolution. In so doing, the importance of the pertinent concepts is enhanced, their scope is enlarged and their utility increased. The whole process enables richer and wider connections in the web of knowledge, embedding theory even deeper in the system's life, revealing more links in the great chain of being!

4.6 Necessary and Best Worlds

In sections 7 through 10 we analyze the role played in modern science by metaphysics, a very special form of heuristic argumentation. Such arguments often explain why a system follows a given trajectory or evolves along a given path. These arguments may explain why a system must follow a necessary path or is effectively forced along a single trajectory; these are "only world" explanations. Teleological arguments explain why a system chooses the best trajectory according to some optimality criterion; these are "best world" explanations. Stochastic or integral arguments explain why the system evolution takes into account, including, averaging, summing or integrating over, all possible or admissible trajectories; these are "possible worlds" explanations.

In sections 7 to 9 we also try to examine the interrelations between "only world", "best world" and "possible worlds" forms of explanation, as well as their role and purpose in the light of cognitive constructivism, since they are at the core of modern metaphysics. We begin this journey by studying in this section a simple and seemingly innocent mathematical puzzle. The puzzle, which will be solved directly by elementary calculus, is in fact used by Richard Feynman as an allegory to present an important variational problem.

Consider a beach with shore line represented by $x = a$, in the standard Cartesian plane. A lifeguard, at position $(x, y) = (0, 0)$, spots a person drowning at position $(x, y) = (a + b, d)$. While on the athletic track the lifeguard car can run at top speed c, on the

sand it can run at speed c/ν_1. Once in the water, the lifeguard can only swim at speed c/ν_2, $1 < \nu_1 < \nu_2$. Letting $(x, y) = (a, y(a))$ be the point where he enters the water, what is the optimal value $y(a) = z$ if he wants to reach position $(a + b, d)$ as fast as possible?

Since the shortest path in an homogenous medium is a straight line, the optimal trajectory is a broken line, from $(0, 0)$ to (a, z), and then from (a, z) to $(a + b, d)$. The total travel time is $J(z)/c$, where

$$J(z) = \nu_1 \sqrt{a^2 + z^2} + \nu_2 \sqrt{b^2 + (d - z)^2} \ .$$

Since we want $J(z)$ at a minimum, we set

$$\frac{dJ}{dz} = \nu_1 \frac{-2z}{2\sqrt{a^2 + z^2}} + \nu_2 \frac{-2(d - z)}{2\sqrt{b^2 + (d - z)^2}} = 0 \ ,$$

so that, we should have

$$\nu_1 \sin(\theta_1) = \nu_2 \sin(\theta_2) \ .$$

Professional lifeguards claim that this simple model can be improved by dividing the sand in a dry band, V_1, and a wet band, V_2, and the water in a shallow band, V_3, and a deep band, V_4, with respective different media 'resistance' indices, $\nu_1, \nu_2, \nu_3, \nu_4$, satisfying $\nu_4 > \nu_3 > \nu_1 > \nu_2 > 1$. Although the solution for the improved model can be similarly obtained, a general formalism to solve 'variational' problems of this kind exists which is known as the Euler-Lagrange equation. For an instructive introduction see Krasnov et al. (1973), Leech (1963) and Marion (1970).

The trigonometric relation, $\nu(x) \sin(\theta) = K$, obtained in the last equation, is known in optics as Snell-Descartes' law. It explains the refraction (bending) of a light ray incident to a surface separating two distinct optic media. In this relation, ν is the medium refraction index. The variational problem solved above was proposed by Pierre de Fermat in 1662 to 'explain' Snell-Descartes' law. Fermat's *principle of least time* states that a ray of light, going from one point to another, follows the path which is traversed in the smallest time.

Notice that Fermat enounced this principle *before* any measurement of the speed of light. The first quantitative estimate of the speed of light, in sidereal space, was obtained by O. Roemer in 1676. He measured the Doppler effect on the period of Io, a satellite of Jupiter discovered by Galileo in 1610. More precisely, he measured the violet and red shifts, i.e., the variation for shorter and longer in the observed periods of Io, as the Earth traveled in its orbit towards and away from Jupiter. Roemer's final estimate was $c = 1au/11'$, that is, one astronomial unit (the length of the semi-major axis of the earth's elliptical orbit around the sun, approximately 150 million kilometres) per 11 minutes. Today's value is around $1au/8'20''$. The first direct measurements of the comparative speed of light in distinct material media (air and water) were obtained by Léon J.B.Foucault, almost two centuries latter, in 1850, using a rotating mirror device.

For details, see Tobin (1993) and Jaffe (1960). For a historical perspective of several competing theories of light we refer to Ronchi (1970) and Sabra (1981).

Snell-Descartes' "law" is an example of mathematical model that dictates a "necessary world", stating, plain and simple, how things "have to be". In contrast, Fermat's "principle" is a theoretical construct that elects a "best world" according to some criterion used to compare "possible worlds".

Fermat's principle is formulated minimizing the integral of $ds = 1/dt$. In a similar way, Leibniz, Euler, Mauperius, Lagrange, Jacobi, Hamilton, and many others were able to reformulate Newtonian mechanics, minimizing the integral of a quantity called *action*, $ds = L\, dt$, where the Lagrangian, L, is the difference between the kinetic energy (Leibniz' vis viva), $(1/2)mv^2$, and the potential energy of the system (Leibniz' vis morta). Hence, these formulations are called in physics principles of minimum action or principles of least action.

4.7   Efficient and Final Causes

At the XVII century, several models of light and its propagation were developed to explain Snell-Descartes' law, see Sabra (1981). The discussion of these models, and the necessary versus best world formulations of optics and mechanics discussed in the last section are historically connected to the discussion of the metaphysical concepts of efficient and final causes.

This terminology dates back to Aristotle, who distinguishes, in Metaphysics, four forms of causation, that is, four types of answers that can be given to a Why-question. Namely:

- Material cause: Because it is made of, or its constituent parts are ...

- Formal cause: Because it has the form of, or is shaped like ...

- Efficient cause: Because it is produced, or accomplished by ...

- Final cause: Because it is intended to, or has the purpose of ...

Efficient and final causes are the subject of this section. For a general overview of the theme in the history of 17th and 18th century Physics, see Brunet (1938), Dugas (1988), Pulte (1989), Goldstine (1980), Wiegel (1986) and Yourgrau and Mandelstam (1979).

Newtonian mechanics is formulated only in terms of efficient causes - an existing force acts on a particle (or body) producing a movement described by the Newtonian differential equations. Least action principles, on the other hand, are formulated through the use of a final cause: the trajectory followed by the particle (or light ray) is that which optimizes a certain characteristic, given its original and final positions. This is why these formulations are also called teleological, from the Greek $\tau\epsilon\lambda o\varsigma$, aim, goal or purpose. A

general discussion of teleological principles in this context was presented by Leibniz in his *Specimen Dynamicum* of 1695, a translation of which appears in Loemker (1969, p.442).

> *"In fact, as I have shown by the remarkable example of the principles of optics, ...(that) final causes may be introduced with great fruitfulness even into the special problems of physics, not merely to increase our admiration for the most beautiful works of the supreme Author, but also to help us make predictions by means of them which could not be as apparent, except perhaps hypothetically, through the use of efficient cause... It must be maintained in general that all existent facts can be explained in two ways - through a kingdom of power or efficient causes and through a kingdom of wisdom or final causes... Thus these two kingdoms everywhere permeate each other, yet their laws are never confused and never disturbed, so the maximum in the kingdom of power, and the best in the kingdom of wisdom, take place together."*

Euler and Maupertuis generalized the arguments of Fermat and Leibniz, deriving Newtonian mechanics from the least action principle.The Principle of Least Action, was stated in Maupertuis (1756, IV, p.36), as his *Lois du Mouvement, Principe Général*,

> *"Laws of Movement, General Principle:*
> *When a change occurs in Nature, the quantity of action necessary for that change is as small as possible.*
> *The quantity of action is the product of the mass of the bodies times their speed and the distance they travel. When a body is transported from one place to another, the action is proportional to the mass of the body, to its speed and to the distance over which it is transported."*

Maupertuis also used the same theological arguments of Leibniz regarding the harmony between efficient and final causes. In Maupertuis (1756, IV, p.20-23 of *Accord de Différents Lois de la Nature, qui avoient jusqu'ici paru incompatibles*), for example, we find:

> *"Accord Between Different Laws of Nature, that seemed incompatible. ...*
> *I know the distaste that many mathematicians have for final causes applied to physics, a distaste that I share up to some point. I admit, it is risky to introduce such elements; their use is dangerous, as shown by the errors made by Fermat (and Leibniz(?)) in following them. Nevertheless, it is perhaps not the principle that is dangerous, but rather the hastiness in taking as a basic principle that which is merely a consequence of a basic principle.*
> *One cannot doubt that everything is governed by a supreme Being who has imposed forces on material objects, forces that show his power, just as he has fated those objects to execute actions that demonstrate his wisdom. The*

harmony between these two attributes is so perfect, that undoubtedly all the effects of Nature could be derived from each one taken separately. A blind and deterministic mechanics follows the plans of a perfectly clear and free Intellect. If our spirits were sufficiently vast, we would also see the causes of all physical effects, either by studying the properties of material bodies or by studying what would most suitable for them to do.

The first type of studies is more within our power, but does not take us far. The second type may lead us stray, since we do not know enough of the goals of Nature and we can be mistaken about the quantity that is truly the expense of Nature in producing its effects.

To unify the certainty of our research with its breadth, it is necessary to use both types of study. Let us calculate the motion of bodies, but also consult the plans of the Intelligence that makes them move.

It seems that the ancient philosophers made the first attempts at this sort of science, in looking for metaphysical relationships between numbers and material bodies. When they said that God occupies himself with geometry, they surely meant that He unites in that science the works of His power with the perspectives of His wisdom."

Some of the metaphysical explanation given by Leibniz and Maupertuis are based on theological arguments which can be regarded as late inheritances of medieval philosophy. This form of metaphysical argument, however, faded away from the mainstream of science after the 18th century. Nevertheless, in the following century, the (many variations of the) least action principle disclosed more powerful formalisms and found several new applications in physics. For details, see Goldstine (1980) and Wiegel (1986). As stated in Yourgrau and Mandelstam (1979, ch.14 of *The Significance of Variational Principles in Natural Philosophy*),

"Towards the end of the (XIX) century, Helmholtz invoked, on purely scientific grounds, the principle of least action as a unifying scientific natural law, a 'leit-motif' dominating the whole of physics, Helmholtz (1887).

'From these facts we may even now draw the conclusion that the domain of validity of the principle of least action has reached far beyond the boundaries of the mechanics of ponderable bodies. Maupertuis' high hopes for the absolute general validity of his principle appear to be approaching their fulfillment, however slender the mechanical proofs and however contradictory the metaphysical speculation which the author himself could at the time adduce in support of his new principle. Even at this stage, it can be considered as highly probable that it is the universal law pertaining to all processes in nature. ... In any case, the general validity of the principle of least action seems to me assured, since it may claim a higher place as a heuristic and guiding principle

in our endeavor to formulate the laws governing new classes of phenomena. Helmholtz (1887).' "

4.8   Modern Metaphysics

In this section we continue the investigation on the use and nature of metaphysical principles in theoretical Physics. Like many others adjectives, the word metaphysical has acquired both a positive (meliorative, eulogistic, appreciative) and a negative (pejorative, derogatory, unappreciative) connotation.

Logical positivism or logical empiricism was a mainstream school in the philosophy of science of the early 20th century. One of the objectives of the positivist school was to build science from empirical (observable) concepts only. According to this point of view every metaphysical, that is, non-empirical or non-directly observable, entity is cognitively meaningless and all teleological principles were perceived to fall in this category.

Teleological arguments were also perceived as problematic in Biology and related fields due to the frequent abuse of phony teleological arguments, usually in the form of crude fallacies or obvious tautologies, given to provide support to whatever statement in need. Maupertuis, the proponent of the first general least action principle, himself, was aware of such problems, as clearly stated in the text of his quoted in the previous section. Why then did important theoretical physicists insist in keeping teleological arguments and other kinds of principles perceived as metaphysical among the regular tools of the trade?

Yourgrau and Mandelstam (1979, p.10) emphasize the heuristic importance of metaphysical principles in the early development of prominent physical theories:

> *"In conformity with the scope of our subject, the speculative facets of the thinkers under review have been emphasized. Historically by far more consequential were the positive contributions to natural science, contributions which transferred the emphasis from 'a priori' reasoning to theories based upon observation and experiment. Hence, while the future exponents of least principles may have been guided in their metaphysical outlook (1) by the idealistic background we have described, they had, nevertheless, to present their formulations in such fashion that the data of experience would thus be explained. A systematic scrutiny of the individual chronological stages in the evolution of minimum principles can furnish us with profound insight into continuous transformation of a metaphysical canon to an exact natural law.*
>
> *(1) By 'metaphysical outlook' we comprehend nothing but those general assumptions which are accepted by the scientist."*

The definition of Metaphysics used by Yougrau is perhaps a bit too vague, or too

humble. We believe that a deeper understanding of the role played by metaphysics in modern theoretical physics can be found (emphases are ours) in Einstein (1950):

> *"We have become acquainted with concepts and general relations that enable us to comprehend an immense range of experiences and make them* **accessible to mathematical treatment***. ...*
>
> *(but) Why do we devise theories at all? The answer to the latter question is simply: Because we enjoy* **comprehending***, i.e., reducing phenomena by the process of logic to something already known or (apparently) evident. ...*
>
> *This is the striving toward* **unification and simplification of the premises of the theory** *as a whole (Mach's principle of economy, interpreted as a logical principle). ...*
>
> *There exists a passion for comprehension, just as there exists a passion for music. That passion is rather common in children, but gets lost in most people later on. Without this passion, there would be neither mathematics nor natural science. Time and again the passion for understanding has led to the illusion that man is able to comprehend the objective world rationally, by pure thought, without any empirical foundations-in short, by metaphysics. I believe that every true theorist is a kind of tamed metaphysicist, no matter how pure a 'positivist' he may fancy himself. The metaphysicist believes that the logically simple is also the real. The tamed metaphysicist believes that not all that is logically simple is embodied in experienced reality, but that the totality of all sensory experience can be 'comprehended' on the basis of a conceptual system built on premises of great simplicity. The skeptic will say that this is a 'miracle creed.' Admittedly so, but it is a miracle creed which has been borne out to an amazing extent by the development of science."*

Even more resolute statements are made by Max Planck (emphases are ours) in the encyclopedia Die Kultur der Gegenwart (1915, p.68), and in Planck (1915, p.71-72):

> *"As long as there exists physical science, its highest desirable goal had been the solution of the problem to* **integrate all natural phenomena** *observed and still to be observed into a* **single simple principle** *which* **permits to calculate** *all past and, in particular, all future processes from the present ones. It is natural that this goal has not been reached to date, nor ever will it be reached entirely. It is well possible, however, to approach it more and more, and the history of theoretical physics demonstrates that on this way a rich number of important successes could already be gained; which clearly indicates that this ideal problem is not merely utopical, but eminently fertile. Among the more or less general laws which manifest the achievements of physical science in the course of the last centuries, the Principle of Least Action is probably the*

one which, as regards form and content, may claim to come nearest to that final ideal goal of theoretical research."

"Who instead seeks for higher connections within the system of natural laws which are most easy to survey, in the interest of the aspired harmony will, from the outset, also admit those means, such as reference to the events at later instances of time, which are not utterly necessary for the complete description of natural processes, but which are **easy to handle** *and can be* **interpreted intuitively***."*

From the last quoted statements of Einstein and Planck we can draw the following four points list of motivations for the use of (or for defining the characteristics of) good metaphysical principles:

1- Simplicity;   2- Generality;   3- Interpretability; and

4- Derivation of powerful and easy to handle (calculate, compute) symbolic (mathematical) formalisms.

The first three these points are very similar to the characteristics of good metaphorical arguments, as analyzed in section 3. In this particular context, generality means the ability of crossing over different areas or transferring knowledge between multiple fields to integrate the understanding of different natural phenomena. Since the least action principle clearly conforms with all four criteria in the above list, it is easy to understand why it is so endeared by physicists, despite the objections to its teleological nature.

Up to this point we have been arguing that the laws of mechanics in integral form, stated in terms of the least action principle, and its associated teleological metaphysical concepts, should be accepted along side with the "standard" formulation of mechanics in differential form, that is, the differential equations of Newtonian mechanics. However, Schlick (1979, V.1, p.297) proposes a complete inversion of the empirical / metaphysical status of the two formulations, see also Muntean (2006) and Stöltzner (2003). According to Schlick's view, while the integral or macro-law formulation has its grounds in observable quantities, the differential or micro-law formulation is based on non-empirical concepts:

"That the event at a point depends only on those processes occurring in its immediate temporal and special neighborhood, is expressed in the fact that space and time appear in the formulae of natural laws as infinitely small quantities; these formulae, that is, are differential equations. We can also describe them in a readily intelligible terminology as micro-laws*. Through the mathematical process of integration, there emerge from them the* macro-laws *(or integral laws), which now state natural dependencies in their extension over spatial and temporal distances. Only the latter fall within experience, for the infinitely small is not observable. The differential laws prevailing in nature can therefore be conjectured and inferred only from the integral laws, and these inferences*

are never, strictly speaking, univocal, since one can always account for the observed macro-laws by various hypotheses about the underlying micro-laws. Among the various possibilities we naturally choose that marked by the greatest simplicity. It is the final aim of exact science to reduce all events to the fewest and simplest possible differential laws."

From this and other examples presented in sections 6 to 9, we come to the conclusion that metaphysical concepts are unavoidable, regardless of the formulation in use. Positivists, on the other hand, envision the exclusive use of metaphysical free scientific concepts, with grounds on pure empirical experience. At the end, it seems that the later devote themselves to the worthless pursuit of chasing chimeras. Moreover, metaphysical arguments are essential to build our intuition. Without intuition, physical reasoning would be downgraded to merely cranking the formalism, either by algebraic manipulation of the symbolic machinery or by sheer number crunching. Planck (1950, p.171-172), states that:

"To be sure, it must be agreed that the positivistic outlook possesses a distinctive value; for it is instrumental to a conceptual clarification of the significance of physical laws, to a separation of that which is empirically proven from that which is not, to an elimination of emotional prejudices nurtured solely by customary views, and it thus helps to clear the road for the onward drive of research. But Positivism lacks the driving force for serving as a leader on this road. True, it is able to eliminate obstacles, but it cannot turn them into a productive factors. For its activity is essentially critical, its glace is directed backward. But progress, advancement requires new associations of ideas and new queries, not based on the results of measurements alone, but going beyond them, and toward such things the fundamental attitude of Positivism is one of aloofness.

Therefore, up to quite recently, positivists of all hues have also put up the strongest resistance to the introduction of atomic hypotheses .... "

At this point it is opportune to remember Kant's allegory of breathing, that offers a couterpoint in contrast and complement to his allegory of the dove (Prolegomena to Any Future Metaphysics; How Is Metaphysics Possible As a Science?):

"That the human mind will ever give up metaphysical researches is as little to be expected as that we should prefer to give up breathing altogether, to avoid inhaling impure air."

4.9 Averaging over All Possible Worlds

The last example quoted by Planck provides yet another excellent illustration to enlighten not only the issue currently under discussion, but also other topics we want to address. In the next section we shortly introduce one of the most important models related to the debate concerning the atomic hypothesis, namely, Brownian motion.

We are interested in the Dirichlet problem of describing the steady state temperature at a two dimensional plate, given the temperature at its border. The partial differential equation that the temperatures, $u(x, y)$, must obey in the Dirichlet problem is known as the 2-dimensional Laplace equation,

$$\text{div grad } u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \ ,$$

as in Butkov (1968, Ch.8).

From elementary calculus, see Demidovich and Maron (1976), we have the forward and backward finite difference approximations for a partial derivative,

$$\frac{\partial u}{\partial x} \approx \frac{u(x + h, y) - u(x, y)}{h} \approx \frac{u(x, y) - u(x - h, y)}{h} \ .$$

Using these approximations twice, we obtain the symmetric or central finite difference approximation for the second derivatives,

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{u(x + h, y) - 2u(x, y) + u(x - h, y)}{h^2} \ ,$$

$$\frac{\partial^2 u}{\partial y^2} \approx \frac{u(x, y + h) - 2u(x, y) + u(x, y - h)}{h^2} \ .$$

Substitution in the Laplace equation gives the "next neighbors' mean value" equation,

$$u(x, y) = \frac{1}{4} \left(u(x + h, y) + u(x - h, y) + u(x, y + h) + u(x, y - h) \right) \ .$$

From the last equation we can set a linear system for the temperatures in a rectangular grid. The unknown variables, in the left hand side, are the temperatures at the interior points of the grid, in the right hand side we have the known temperatures at the boundary points.

From the temperatures at the four neighboring points of a given grid point, $[x, y]$, an estimate of the temperature, $u(x, y)$, at this point is the expected value of the random variable $Z(x, y)$ whose value is uniformly sampled from

$$\{u(x + h, y), u(x - h, y), u(x, y + h), u(x, y - h)\} \ ,$$

the north, south, east and west neighbors. Also, if we did not know the temperature at the neighboring point sampled, we could estimate the neighbor's temperature by sampling

one of the neighbor's neighbors. Using this argument recursively, we could estimate the temperature $u(x, y)$ through the following Monte Carlo algorithm:

Consider a "particle" undergoing a symmetric random (or drunken sailor) walk, that is, a stochastic trajectory, $T = [T(1), \ldots T(m)]$, such that starting at position $T(1) = [x(1), y(1)]$, it jumps to positions $T(1), T(2), \ldots T(m)$ by uniformly sampling among the neighboring points of its current position, until it eventually hits the boundary. More precisely, from a given position, $T(k) = [x(k), y(k)]$, at step k, the particle will equally likely jump to one of its neighboring positions at step $k + 1$, that is,

$$T(k + 1) = [x(k + 1), y(k + 1)]$$

is randomly selected from the set

$$\{ [x(k) + h, y(k)], [x(k) - h, y(k)], [x(k), y(k) + h], [x(k), y(k) - h] \} .$$

The journey ends when a boundary point, $T(m) = [x(m), y(m)]$, is hit by "particle" at (random) step m. Defining the random variable $Z(T) = u(x(m), y(m))$, it can be shown that the expected value of $Z(T)$, for T starting at $T(1) = [x(1), y(1)]$, equals $u(x(1), y(1))$, the solution to the Dirichlet problem at $[x(1), y(1)]$.

The above algorithm is only a particular case of more general Monte Carlo algorithms for solving linear systems. For details see Demidovich and Maron (1976), Hammersley and Handscomb (1964), Halton (1970) and Ripley (1987). Hence, these Monte Carlo algorithms allow us to obtain the solution of many continuous problems in terms of an expected (average) value of a discrete stochastic flow of particles. More precisely, efficient Monte Carlo algorithms are available for solving linear systems, and many of the mathematical models in Physics, or science in general, are (or can be approximated by) linear equations. Consequently, one should not be surprised to find physical models interpretations in terms of particle flows.

In 1827, Robert Brown observed the movement of plant spores (pollen) immersed in water. He noted that the spores were in perpetual movement, following an erratic or chaotic path. Since the motion persisted over long periods of time on different liquid media and powder particles of inorganic minerals also exhibited the same motion pattern, he discarded the hypothesis of live or self propelled motion. This "Brownian motion" was the object of several subsequent studies, linking the intensity of the motion to the temperature of the liquid medium. For further readings, see Brush (1968) and Haw (2002).

In 1905 Einstein published a paper in which he explains Brownian motion as a fluctuation phenomenon caused by the collision of individual water molecules with the particle in suspension. Using a simplified argument, we can model the particle's motion by a random path in a rectangular grid, like the one used to solve the Dirichlet problem. In this model, each step is interpreted as a molecule collision with the particle, causing it to move, equally likely, to the north, south, east or west. The stating the formal mathematical properties of this stochastic process, known as a random walk, was one of the

many scientific contribution of Norbert Wiener, one of the forefathers of Cybernetics, see Wiener (1989). For good reviews, see Beran (1994) and Embrechts (2002). For an elementary introduction, see Berg (1993), Lemons (2002) MacDonald (1962) and Mikosch (1998).

A basic assumption of the random walk model is that distinct collisions or moves made by the particle are uncorrelated. Let us consider the one dimensional random walk process, where a particle, initially positioned at the origin, $y_0 = 0$, undergoes incremental unitary steps, that is, $y_{t+1} = y_t + x_t$, and $x_t = \pm 1$. The steps are assumed unbiased, and uncorrelated, that is, $E(x_t) = 0$ and $\text{Cov}(x_s, x_t) = 0$. Also, $\text{Var}(x_t) = 1$. From the linearity of the expectation operator, we conclude that $E(y_t) = 0$. Also

$$E(y_t^2) = E\left(\sum_{j=1}^{t} x_j\right)^2 = E\sum_{j=1}^{t} x_j^2 + E\sum_{j\neq k} x_j x_k = t + 0 = t \ ,$$

so that at time t, the standard deviation of the particle's position is

$$\sqrt{E(y_t^2)} = t^H, \text{ for } H = \frac{1}{2} \ .$$

From this simple model an important characteristic, expressed as a sharp statistical hypothesis to be experimentally verified, can be derived: Brownian motion is a self-similar process, with scaling factor, or Hurst exponent, $H = 1/2$. One possible interpretation of the last statement is that, in other to make coherent observations of a Brownian motion, if time is rescaled by a factor ϕ, then space should also be rescaled by a factor ϕ^H. The generalization of this stochastic process for $0 < H < 1$, is known as fractional Brownian motion.

The sharp hypothesis $H = 1/2$ takes us back to the eternal underlying theme of system coupling / decoupling. While regular Brownian motion was built under the essential axiom of decoupled (uncorrelated) increments over non-overlapping time intervals, the relaxation of this condition, without sacrificing self-similarity, leads to long range correlations. For fresh insight, see the original work of Paul Levy (1925, 1948, 1954, 1970) and Benoît Mandelbrot (1983); for a textbook, see Beran (1994) and Embrechts (2002).

As we have seen in this section, regular Brownian motion can be very useful in modeling the low level processes often found in disorganized physical systems. However, in several phenomena related to living organisms or systems, long range correlations are exhibited. This is the case, for example, in the study of many complex or (self) organized systems, such as colloids or liquid crystals, found in soft matter science, in the development of embryos or social and urban systems, in electrocardiography, electroencephalography or other monitoring of biological signals procedures. Modeling in many of these areas can, nevertheless, benefit from the techniques of fractional Brownian motion, as seen in Addison (1997), Beran (1994), Bunde and Havlin (1994), Embrechts (2002) and Feder (1988). Some of the epistemological consequences of the mathematical and computational models introduced in this section are commented in the following section.

4.10   Hypothetical versus Factual Models

The Monte Carlo algorithms introduced in the last section are based on the stochastic flow of particles. Yet, these particles can be regarded as mere imaginary entities in a computational procedure. On the other hand, some models based on similar ideas, such as the kinetic theories of gases, or the random walk model for the Brownian motion, seem to give these particles a higher ontological status. It is thus worthwhile to discuss the epistemological or ontological status of an entity in a computational procedure, like the particles in the above example.

This discussion is not as trivial, innocent and harmless, at it may seem at first sight. In 1632 Galileo Galilei published in Florence his Dialogue Concerning the Two Main World Systems. At that time it was necessary to have a license to publish a book, the *imprimatur*. Galileo had obtained the imprimatur from the ecclesiastical authorities two years earlier, under the explicit condition that some of the theses presented in the book, dangerously close to the heliocentric heretical ideas of Nicolas Copernicus, should be presented as a "hypothetical model" or as a "calculation expedient" as opposed to the "truthful" or "factual" description of "reality".

Galileo not only failed to fulfill the imposed condition, but also ridiculed the official doctrine. He presented his theories in a dialogue form. In these dialogues, Simplicio, the character defending the orthodox geocentric ideas of Aristotle and Ptolemy, was constantly mocked by his opponent, Salviati, a zealot of the views of Galileo. In 1633 Galileo was prosecuted by the Roman Inquisition, under the accusation of making heretical statements, as quoted from Santillana (1955, p.306-310):

> *"The proposition that the Sun is the center of the world and does not move from its place is absurd and false philosophically and formally heretical, because it is expressly contrary to Holy Scripture. The proposition that the Earth is not the center of the world and immovable but that it moves, and also with a diurnal motion, is equally absurd and false philosophically and theologically considered at least erroneous in faith."*

In the Italian renaissance, one of the most open and enlighten societies of its time, but still within a pre-modern era, where subsystems were only incipient and not clearly differentiated, the consequences of mixing scientific and religious arguments could be daring. Galileo even uses some arguments that resemble the concept of systemic differentiation, for example:

> *"Therefore, it would perhaps be wise and useful advice not to add without necessity to the articles pertaining to salvation and to the definition of faith, against the firmness of which there is no danger that any valid and effective doctrine could ever emerge. If this is so, it would really cause confusion to*

add them upon request from persons about whom not only do we not know whether they speak with heavenly inspiration, but we clearly see they are deficient in the intelligence necessary first to understand and then to criticize the demonstrations by which the most acute sciences proceed in confirming similar conclusions." Finocchiaro (1991, p.97).

The paragraph above is from a letter of 1615 from Galileo to Her Serene Highness Grand Duchess Cristina but, as usual, Galileo's rhetoric is anything but serene. In 1633 Galileo is sentenced to prison for an indefinite term. After he abjures his allegedly heretical statements, the sentence is commuted to house-arrest at his villa. Legend has it that, after his formal abjuration, Galileo muttered the now celebrated phrase,

Eppur si mouve, "But indeed it (the earth) moves (around the sun)".

Around 1610 Galileo built a telescope (an invention coming from Netherland) that he used for astronomical observations. Among his findings were four satellites to planet Jupiter, namely, Io, Europa, Ganymedes and Callisto. He also observed phases (such as the lunar phases) exhibited by planet Venus. Both facts are either compatible or explained by the Copernican heliocentric theory, but problematic or incompatible with the orthodox Ptolemaic geocentric theory. During his trial, Galileo tried to use these observations to corroborate his theories, but the judges would not, literally, even 'look' at them. The church's chief astronomer, Christopher Clavius, refused to look through Galileo's telescope, stating that there was no point in 'seeing' some objects through an instrument that had been made just in order to 'create' them. Nevertheless, only a few years after the trial, the same Clavius was building fine telescopes, used to make new astronomical observations. He took care, of course, not to upset his boss with "theologically incorrect" explanations for what he was observing.

From the late 19th century to 1905 the world witnessed yet another trial, perhaps not so famous, but even more dramatic. Namely, that of the atomistic ideas of Ludwig Boltzmann. For a excellent biography of Boltzmann, intertwined (as it ought to be) with the history of his scientific ideas, see Cercignani (1998). The final verdict on this controversy was given by Albert Einstein in his *annus mirabilis* paper about Brownian Motion, together with the subsequent experimental work of Jean Perrin. For details see Einstein (1956) and Perrin (1950). A simplified version of these models was presented in the previous section, including a "testable" sharp statistical hypothesis, $H = 1/2$, to empirically check the theory. As quoted in Brush (1968), in his Autobiographical Notes, Einstein states that:

"The agreement of these considerations with experience together with Planck's determination of the true molecular size from the law of radiation (for high temperatures) convinced the skeptics, who were quite numerous at that time

(Ostwald, Mach) of the reality of atoms. The antipathy of these scholars towards atomic theory can indubitably be traced back to their positivistic philosophical attitude. This is an interesting example of the fact that even scholars of audacious spirit and fine instinct can be obscured in the interpretation of facts by philosophical prejudices. The prejudice - which has by no means died out in the meantime - consists in the faith that facts themselves can and should yield scientific knowledge without free conceptual construction.

Such misconception is possible only because one does not easily become aware of the free choice of such concepts, which through verification and long usage, appear to be immediately connected with the empirical material"

Let us follow Perrin's perception of the "empirical connection" between the concepts used in the molecular theory, which contrasted to that of the rival energetic theory, during the first decade of the 20th century. In 1903 Perrin was already an advocate of the molecular hypothesis, as can be seen in Perrin (1903). According to Brush (1968, p.30-31), Perrin refused the positivist demand for using only directly observable entities. Perrin referred to an analogous situation in biology where,

"the germ theory of disease might have been developed and successfully tested before the invention of the microscope; the microbes would have been hypothetical entities, yet, as we know now, they could eventually be observed."

But only three years latter, was Perrin (1906) confident enough to reverse the attack, accusing the energetic view rivaling the atomic theory, of having "degenerated into a pseudo-religious cult". It was the energetic theory, claimed Perrin, that was making use of non-observable entities! To begin with, Classical thermodynamics had a differential formulation, with the functions describing the evolution of a system assumed to be continuous and differentiable (notice the similarity between the argument of Perrin and that of Schlick, presented in section 8). Perrin based his argument of the contemporary evolution of mathematical analysis when, until late in the 20th century, continuous functions were naturally assumed to be differentiable. Nevertheless, the development of mathematical analysis, on the turn to the 20th century, proved this to be a rather naive assumption. Referring to this background material, Perrin argues:

"But they still thought the only interesting functions were the ones that can be differentiated. Now, however, an important school, developing with rigor the notion of continuity, has created a new mathematics, within which the old theory of functions is only the study (profound, to be sure) of a group of singular cases. It is curves with derivatives that are now the exception; or, if one prefers the geometrical language, curves with no tangents at any point become the rule, while familiar regular curves become some kind of curiosities, doubtless interesting, but still very special."

In three more years, even former opponents were joining the ranks of the atomic theory. As W.Nernst (1909, 6th.ed., p.212) puts it:

> *"In view of the* ocular *confirmation of the picture which the kinetic theory provides us of the world of molecules, one must admit that this theory begins to lose its hypothetical character."*

4.11   Magic, Miracles and Final Remarks

In several incidents analyzed in the last sections, one can repeatedly find the occurrence of theoretical "phase transitions" in the history of science. In these transitions, we observe a dominant and strongly supported theory being challenged by an alternative point of view. In a first moment, the cheerleaders of the dominant group come up with a variety of "disqualifying arguments", to show why the underdog theory, plagued by phony concepts and faulty constructions, should not even be considered as a serious contestant. In an second moment, the alternative theory is kept alive by a small minority, that is able to foster its progress. In a third and final moment, the alternative theory becomes, quite abruptly, the dominant view, and many wonder how is it that the old, now abandoned theory, could ever had so much support. This process is captured in the following quotation, from the preface to the first edition of Schopenhauer (1818):

> *"To truth only a brief celebration of victory is allowed between the two long periods during which it is condemned as paradoxical, or disparaged as trivial."*

Perhaps this is the basis for the gloomier statement found in Planck (1950, p.33-34):

> *"A new scientific truth does not triumph by convincing its opponents and by making them see the light, but rather because its opponents eventually die, and a new generation grows up that is familiar with it."*

As for the abruptness of the transition between the two phases, representing the two theoretical paradigms, this is a phenomenon that has been extensively studied, from sociological, systemic and historical perspectives, by Thomas Kuhn (1996, 1977). See also Hoyningen-Huene (1993) and Lakatos (1978a,b). For similar ideas presented within an approach closer to the orthodox Bayesian theory, see Zupan (1991).

We finish this section with a quick and simple alternative explanation, possibly just as a hint, that I believe can shed some light on the nature of this phenomenon. Elucidations of this kind were used many times by von Foerster (2003,b,e) who was, among many other things, a skilful magician and illusionist.

An Ambigram, or ambiguous picture, is a picture that can be looked at in two (or more) different ways. Looking at an ambigram, the observer's interpretation or re-solution of the image can be attracted to one of two or more distinct eigen-solutions. A memorable instance of an ambigram is the Duck-Rabbit, born in 1892, in the humble pages of the German tabloid Fliegende Blätter. It was studied in 1899 by the psychologist Joseph Jastrow in an article antecipating several aspects of cognitive constructivism, and finally made famous by the philosopher Ludwig Wittgenstein in 1953. For a historical account of this ambigram, see Kihlstrom (2006), as well as several nice figures. In case anyone wonders, Jastrow was Peirce's Ph.D. student and coauthor of the 1885 paper introducing randomization, and Wittgenstein is no other than von Foster's uncle Ludwig.

According to Jastrow (1899), an ambigram demonstrates how

> *"True seeing, observing, is a double process, partly objective or outward - the thing seen and the retina - and partly subjective or inward - the picture mysteriously transferred to the mind's representative, the brain, and there received and affiliated with other images."*

Still according to Jastrow, in an ambigram,

> *"...a single outward impression changes its character according as it is viewed as representing one thing or another. In general we see the same thing all the time, and the image on the retina does not change. But as we shift the attention from one portion of the view to another, or as we view it with a different mental conception of what the figure represents, it assumes a different aspect, and to our mental eye becomes becomes quite a different thing."*

Jastrow also describes some characteristics of the mental process of shifting between the eigen-solutions of an ambigram, that is, how in *"The Mind's Eye"* one changes from one interpretation to the other. Two of these characteristics are specially interesting in our context:

First, in the beginning, *"It may require a little effort to bring about this change, but it is very marked when once realized."*

Second, after both interpretations are known, *"Most observers find it difficult to hold either interpretation steadily, the fluctuation being frequent, and coming as a surprise."*

The first characteristic can help us understand either Nernst's "ocular readiness" or, in contrast, Clavius' "ocular blindness". After all, the satellites of Jupiter were quite tangible objects, ready to be watched through Galileo's telescope, whereas the grains of colloidal suspension that could be observed with the lunette of Perrin's apparatus provided a much more indirect evidence for the existence of molecules. Or maybe not, after all, it all depends on what one is capable, ready, or willing to see...

The second characteristic can help us understand Leibniz' and Maupertuis' willingness to accommodate and harmonize two alternative explanations for a single phenomenon, that is, to have effective and final causes, or micro and macro versions of physical laws.

Yet, the existence of sharp, stable, separable and composable eigen-solutions for the scientific system in its interaction with its environment, goes far beyond our individual or collective desire to have them there.

These eigen solutions are the basis upon which technology builds much of the world we live in. How well do the eigen-solutions used in these technological gadgets conform with von Foerster criteria? Well, the machine I am using to write this chapter has a 2003 Intel Pentium CPU carved on a silicon waffle with a "precision" of 0.000,000,1m, and is "composed" by about 50 million transistors. This CPU has a clock of 1GHz, so that each and every one of the transistors in this composition must operate synchronously to a fraction of a thousandth of a thousandth of a thousandth of a second!

And how well do the eigen-solutions expressed as fundamental physical constants, upon which technological projects rely, conform with von Foerster criteria? Again, some of these constants are known up to a precision (relative standard uncertainty) of 0.000,000,001, that is, a thousandth of a thousandth of a thousandth! The world wide web site of the United States' National Institute of Standards and Technology, at `www.physics.nist.gov,` gives an encyclopaedic view of these constants and their inter-relations. Planck (1950, Ch.6) comments on their epistemological significance.

But far beyond their practical utility or even their scientific interest, the existence of these eigen-solutions are not magical illusions, but true miracles. Why "true" miracles? Because the more they are explained and the better they are understood, the more wonderful they become!

Chapter 5

Complex Structures, Modularity, and Stochastic Evolution

> *"Hierarchy, I shall argue, is one of the central structural schemes that the architect of complexity uses."*
>
> *"The time required for the evolution of a complex form from simple elements depends critically on the number and distribution of potential intermediate stable subassemblies."*
>
> Herbert Simon (1916-2001),
> The Sciences of the Artificial.

> *"In order to make some sense here, we must keep an open mind about the possibility that for sufficiently complex systems, amplitudes become probabilities.*
>
> Richard Feynman (1918-1988),
> Lecture notes on Gravitation.

5.1   Introduction

The expression *stochastic evolution* may seem an oxymoron. After all, evolution indicates progress towards complexity and order, while a stochastic (probabilistic, random) process seems to be only capable of generating confusion or disorder. The etymology of the word stochastic, from $\sigma\tau o\chi o\varsigma$, meaning *aim*, *goal* or *target*, and its current use, meaning *chancy* or *noisy*, seems to incorporate this apparent contradiction. An alternative use of the same

root, $\sigma\tau o\chi\alpha\sigma\tau\iota\kappa o\varsigma$ meaning *skillful at guessing, conjecturing, or divining the truth*, may offer a bridge between the two meanings.

The main goal of this chapter is to study how the concepts of stochastic process and evolution of complex systems can be reconciled. Sections 2 and 3 examine two prototypical algorithms: Simulated Annealing and Genetic Programming. The ideas behind these two algorithms will be used as a basis for most of the arguments used in this chapter. The mathematical details of some of these algorithms are presented in appendix H. Section 4 presents the concept of modularity, and explains its importance in the evolution of complex systems.

While sections 2, 3 and 4 are devoted to the study of general systems, including applications to biological organisms and technological devices, section 5 pays closer attention to the evolution of complex hypotheses and scientific theories. Section 5 also examines the idea of complementarity, developed by the physicist and philosopher Niels Bohr as a general framework for the reconciliation of two concepts that appear to be incompatible but are, at the same time, indispensable to the understanding of a given system. Section 6 explores the connection between complementarity and probability, presenting Heisenberg's uncertainty principle. Section 7 extends the discussion to general theories of evolution and returns to the pervasive theme of probabilistic causation. Section 8 presents our final remarks.

5.2   The Ergodic Path: One for All

Most human societies are organized as hierarchical structures. Universities are organized in research groups, departments, institutes and schools; Armies in platoons, battalions, regiments and brigades; and so on. This has been the way of doing business as described in the earliest historical records. Deuteronomy (1:15) describes the ancient hierarchical structure of Israel:

> "So I took the heads (ROSh) of your tribes, men wise and known, and made them heads over you, leaders (ShR) of thousands , hundreds, fifties and tens, and officers (ShTR) for your tribes."

This verse gives us some idea of the criteria used to appoint leaders (knowledge and wisdom), but give us no hint on the criteria and methods used to form the groups (of 10, 50, 100 and 1000). Perhaps that was obvious from the family and tribal structure already in place. There are many situations, however, where organizing groups to obtain an optimal structure is far from trivial. In this section we study such a case: the block partition problem.

5.2.1 Block Partitions

The matrix block partition problem arises in many practical situations in engineering design, operations research and management science. In some applications, the elements of a rectangular matrix, A, may represent the interaction between people, corresponding to columns, and activities, corresponding to rows, that is, A_i^j, the element in row i and column j, represents the intensity of the interaction between person j and activity i. The block partition problem asks for an optimal ordering or permutation of rows and columns taking the permuted matrix to Block Angular Form (BAF), so that each one of b diagonal blocks bundles a group of strongly coupled people and activities. Only a small number of activities are leaft outside the diagonal blocks, in a special $(b+1)$-th block of residual rows. Also, only a small number of people interact with more than one of the b diagonal activities, these corespond to residual columns, see Figure 1.

```
┌                                 ┐          ┌                       ┐
│ 1           1 1         1     1 │          │ 1               1  1  │
│ 1 1           1         1 1     │          │ 1  1               1  │
│     1   1     1         1 1 1   │          │       2      2      2 │
│       1   1 1                 1 │          │          2      2  2  │
│ 1 1 1 1 1 1 1           1 1 1   │    ,     │ 3  3  3  3  3  3  3   │
│               2     2 2     2 2 │          └                       ┘
│               2 2     2 2     2 │
│               2 2 2     2 2     │
│ 3     3     3     3     3 3 3 3 │
│   3     3       3 3     3 3 3 3 │
└                                 ┘
```

Figure 1a,b: Two Matrices in Block Angular Form.

A matrix in BAF is in Row Block Angular Form (RBAF) if it has only residual rows, and is in Column Block Angular Form (CBAF) if it has only residual columns. Each angular block can, in turn, exhibit again a BAF, thus creating a recursive or Nested Block Angular Form (NBAF). Figure 1a exhibits a matrix in NBAF. In this figure, zero elements of the matrix are represented by blanck spaces. The number at the position of a non-zero element (NZE) is not the corresponding matrix element's value, but rather a class tag or "color" indicating the block to which the row belongs. Residual rows receive the special color $b+1$. The first block has a nested CBAF structure, shown in Figure 1b. For the sake of simplicity, this chapter will focus on the BAF partition problem, although all our conclusions can be generalized to the NBAF case.

We motivate the block partition problem further with an application related to numerical linear algebra. Gaussian elimination is the name of a simple method for solving linear systems of order n, by reducing the matrix of the original system to (upper) triangular form. This is accomplished by successively subtracting multiples of the row 1 through n from the rows bellow them, so as to eliminate (zero) the elements below each diagonal element (or pivot element). The example in Figure 2 illustrates the Gaussian elimination

algorithm, where the original system, $Ax = b$, is transformed into an upper triangular system, $Ux = c$. The matrix L stores the multipliers used in the process. Each multiplier is stored at the position of the element it was used to eliminate, that is, at the position of the zero it was used to create. It is easy to check that $A = LU$, hence the alternative name of the algorithm: LU Factorization.

The example in Figure 2 also displays some structural peculiarities. Matrix A is in BAF, with two diagonal blocks, one residual row (at the bottom or south side of the matrix) and one residual column (at the right or east side of the matrix). This structure is preserved in the L and U factors. This structure and its preservation is of paramount importance in the design of efficient factorization algorithms. Notice that the elimination process in Figure 2 can be done in parallel. That is, the factorization of each diagonal block can be done independently of and simultaneously with the factorization of the other blocks, for more details see Stern and Vavasis (1994).

$$
\left[\begin{array}{ccc|ccc|c}
1 & 2 & 3 & 0 & 0 & 0 & 1 \\
1 & 6 & 8 & 0 & 0 & 0 & 3 \\
2 & 8 & 17 & 0 & 0 & 0 & 7 \\
\hline
0 & 0 & 0 & 2 & 3 & 4 & 4 \\
0 & 0 & 0 & 4 & 11 & 14 & 13 \\
0 & 0 & 0 & 4 & 16 & 27 & 24 \\
\hline
1 & 10 & 31 & 8 & 37 & 88 & 98
\end{array}\right]
=
\left[\begin{array}{ccc|ccc|c}
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 \\
2 & 2 & 1 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 2 & 1 & 0 & 0 \\
0 & 0 & 0 & 2 & 2 & 1 & 0 \\
\hline
1 & 2 & 3 & 4 & 5 & 6 & 1
\end{array}\right]
\left[\begin{array}{ccc|ccc|c}
1 & 2 & 3 & 0 & 0 & 0 & 1 \\
0 & 4 & 5 & 0 & 0 & 0 & 2 \\
0 & 0 & 6 & 0 & 0 & 0 & 3 \\
\hline
0 & 0 & 0 & 2 & 3 & 4 & 4 \\
0 & 0 & 0 & 0 & 5 & 6 & 5 \\
0 & 0 & 0 & 0 & 0 & 7 & 6 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 7
\end{array}\right]
$$

Figure 2: A=LU Factorization of CBAF Matrix

A classic combinatorial formulation for the CBAF partition problem, for a rectangular matrix A, m by n, is the Hypergraph Partition Problem (HPP). In the HPP formulation, we paint all nonzero elements (NZE's) in a vertex $i \in \{1, \ldots, m\}$, (corresponding to row A_i) with a color $x_i \in \{1, \ldots, b\}$. The color $q^j(x)$ of an edge $j \in \{1, \ldots, n\}$, (corresponding to column A^j) is then the set of all its NZE's colors. Multicolored edges of the hypergraph (corresponding to columns of the matrix containing NZE's of several colors) are the residual columns in the CBAF. The formulation for the general BAF problem also allows some residual rows to receive the special color $b + 1$.

The BAF applications typically require:
1. Roughly the same number of rows in each block.
2. Only a few residual rows or columns.
From 1 and 2 it is natural to consider the minimization of the objective or cost function

$$
f(x) = \alpha \sum_{k=1}^{b} h_k(x)^2 + \beta c(x) + \gamma r(x) \ , \quad h_k(x) = s_k(x) - m/b \ ,
$$

$$
q^j(x) = \left\{ k \in \{1, \ldots, b\} \ : \ \exists i, \ A_i^j \neq 0 \wedge x_i = k \right\} \ , \quad s_k(x) = |\{i \in \{1, \ldots, m\} \ : \ x_i = k\}| \ ,
$$

$$
c(x) = \left|\left\{ j \in \{1, \ldots, n\} \ : \ |q^j(x)| \geq 2 \right\}\right| \ , \quad r(x) = |\{i \in \{1, \ldots, m\} \ : \ x_i = b + 1\}| \ .
$$

The term $c(x)$ is the number of residual columns, and the term $r(x)$ is the number of residual rows. The constraint functions $h_k(x)$ measure the deviation of each block from the ideal size m/b. Since we want to enforce these constraints only approximately, we use quadratic penalty functions, $h_k(x)^2$, that (only) penalize large deviations. If we wanted to enforce the constraints more strictly, we could use exact penalty functions, like $|h_k(x)|$, that penalize even small deviations, see Bertzekas and Tsitsiklis (1989) and Luenberger (1984).

5.2.2   Simulated Annealing

The HPP stated in the last section is very difficult to solve exactly. Technically it is an NP-hard problem, see Cook (1997). Consequently, we try to develop heuristic procedures to find approximate or almost optimal solutions. Simulated Annealing (SA) is a powerful meta-heuristic, well suited to solve many combinatorial problems. The theory behind SA also has profound epistemological implications, that we explore latter on in this chapter.

The first step to define an SA procedure is to define a neighborhood structure in the problem's state or configuration space. The neighborhood, $N(x)$, of a given initial state, x, is the set of states, y, that can be reached from x, by a single move. In the HPP, a single move is defined as changing the color of a single row, $x_i \longmapsto y_i$.

In this problem, the neighborhood size is therefore the same, for any state x, namely, the product of the number of rows and colors, that is, $|N(x)| = mb$ for CBAF, and $|N(x)| = m(b+1)$ for BAF. This neighborhood structure provides good mobility in the state space, in the sense that it is easy to find a path (made by a succession of single moves) from any chosen initial state, x, to any other final state, y. This property is called irreducibility or strong connectivity. There is also a second technical requirements for good mobility, namely, this set of paths should be aperiodic. If the length (the number of single moves) of any path from x to y is a multiple of an integer $k > 1$, k is called the period of this set. Further details are given in appendix H.1.

In an SA, it is convenient to have an easy way to update the cost function, computed at a given state, x, to the cost of a neighboring state, y. The column color weight matrix, W, is defined so that the element W_k^j counts the number of NZE's in column j (in rows) of color k, that is,

$$W_k^j \equiv \left| \left\{ A_i^j \mid A_i^j \neq 0 \wedge x_i = k \right\} \right| \ .$$

The weight matrix can be easily updated at any single move and, from W, it is easy to compute the cost function or a cost differential,

$$\delta \equiv f(y) - f(x) \ .$$

The internal loop of the SA is a Metropolis sampler, where single moves are chosen at random (uniformly among any possible move) and then accepted with the Metropolis

probability,

$$M(\delta, \theta) \equiv \begin{cases} 1, & \text{if } \delta \le 0 ; \\ \exp(-\theta \, \delta), & \text{if } \delta \ge 0 . \end{cases}$$

The parameter θ is known as the inverse temperature, which has a natural interpretation in statistical physics, see MacDonald (2006), Nash(1974) and Rosenfeld (2005), for intuitive introductions, and Thompson (1972) for a rigorous text.

The Gibbs distribution, $g(\theta)^x$, is the invariant distribution for the Metropolis sampling process, given by

$$g(\theta)^x = \frac{1}{Z(\theta)} \exp(-\theta f(x)) \quad \text{with} \quad Z(\theta) = \sum_x \exp(-\theta f(x)) .$$

The symbol $g(\theta)$ represents a row vector, where the column index, x, spans the possible states of the system.

Consider a system prepared (shuffled) in such a way that the probability of starting the system in initial state x is $g(\theta)^x$. If we move the system to a neighboring state, y, according to the Metropolis sampling procedure, the invariance property of the Gibbs distribution assures that the probability that the system will land (after the move) in any given state, y, is $g(\theta)^y$, that is, the probability distribution of the final (after the move) state remains unchanged.

Under appropriate regularity conditions, see appendix H.1, the process is also ergodic. Ergodicity means that even if the system is prepared (shuffled) with an arbitrary probability distribution, $v(0)$, for the initial state, for example, the uniform distribution, the probability distribution, $v(t)$, of the final system state after t moves chosen according to the Metropolis sampling procedure will be sufficiently close to $g(\theta)$ for sufficiently large t. In other words, the probability distribution of the final system state converges to the process' invariant distribution. Consequently, we can find out the process' invariant distribution by following, for a long time, the trajectory of a single system evolving according to to the Metropolis sampling procedure. Hence the expression, The Ergodic Path: One for All. From the history of an individual system we can recover important information about the whole process guiding its evolution.

Let us now study how the Metropolis process can help us finding the optimal (minimum cost) configuration for such a system. The behavior of the Gibbs distribution, $g(\theta)$, changes according to the inverse temperature parameter, θ:
- In the high temperature extreme, $1/\theta \to \infty$, the Gibbs distribution approaches the uniform distribution.
- In the low temperature extreme, $1/\theta \to 0$, the Gibbs distribution is concentrated in the states with minimum cost only.

Correspondingly the Metropolis process behaves as follows:
- At the high temperature extreme, the Metropolis process becomes insensitive to the

value of the cost function, wandering (uniformly) at random in the state space.
- At the low temperature extreme, the Metropolis process becomes very sensitive to the value of the cost function, accepting only downhill moves, until it reaches a local optimum.

The central idea of SA involves the use intermediate temperatures:
- At the beginning use high temperatures, in order to escape the local optima, see Figure 3a (L), placing the process at the deepest valley, and
- At the end use low temperatures, in order to converge to the global optimum (the local optimum at the deepest valley), see Figure 3a (G).
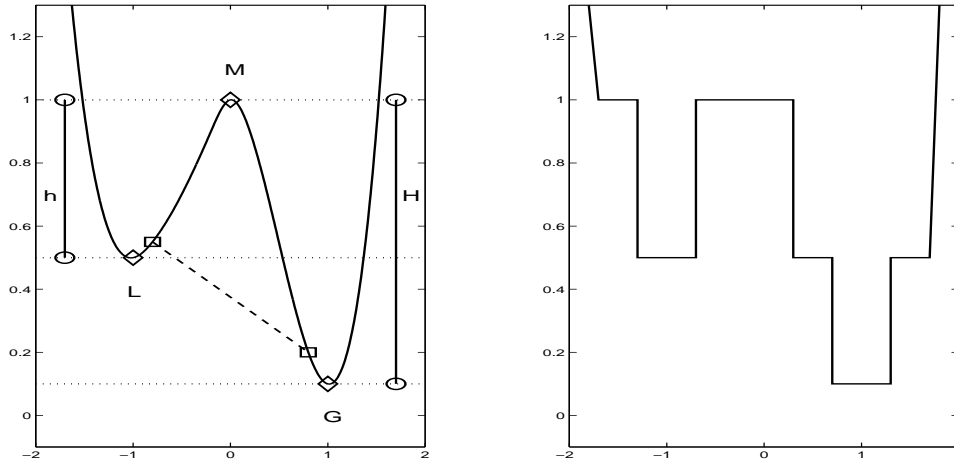
Figure 3a: L,G- Local and global minimum; M- Maximum;
S- Short-cut; h,H- Local and global escape energy.
Figure 3b: A difficult problem, with steep cliffs and flat plateaus.

The secret to play this trick is in the external loop of the SA algorithm, the Cooling Schedule. The cooling schedule initiates the temperature high enough so that most of the proposed moves are accepted, and then slowly cools down the process, until it freezes at an optimum state. The theory of SA is presented in appendix H.1.

The most important result concerning the theory of SA, states that, under appropriate regularity conditions, the process converges to the system's optimal solution as long as we use the Logarithmic Cooling Schedule. This schedule draws the t-th move according to Metropolis process using temperature

$$\theta(t) = \frac{1}{n\Delta} \ln(t) \ ,$$

where Δ is the maximum objective function differential in a single move and n is the minimum number of steps needed to connect any two states. Hence, the *cooling constant*, $n\Delta$ can be interpreted as an estimate of how high a mountain we may need to climb in order to reach the optimal position, see Figure 3a(h).

Practical implementations of SA usually cool the temperature geometrically, $\theta \leftarrow (1 + \epsilon)\theta$, after each batch of Metropolis sampling. The SA is terminated when it freezes, that is, when the acceptance rate in the Metropolis sampling drops below a pre-established threshold. Further details on such an implementation are given in the next section.

5.2.3   Heuristic Acceleration

The Standard Simulated Annealing (SSA), described in the last section, behaves poorly in the BAF problem mainly because it is very difficult to sense the proximity of low cost states, see Figure 3b, that is,

1. Most of the neighbors of a low cost state, x, may have much higher costs; and

2. The problem is highly degenerate in the sense that there are states, x, with a large (sub) neighborhood of equal cost states, $S(x) = \{y \in N(x) \,|\, f(y) = f(x)\}$. In this case, even rejecting all the proposals that would take us out of S, would still give us a significant acceptance rate.

Difficulty 2, in particular, implies the failure of the SSA termination criterion: A degenerate local minimum (or meta-stable minimum) could trap the SSA into forever, sustaining an acceptance rate above the established threshold.

The best way we found to overcome these difficulties is to use a heuristic temperature-dependent cost function, designed to accelerate the SA convergence to the global optimum and to avoid premature convergence to locally optimal solutions:

$$f(x, \mu(\theta)) \equiv f(x) + \frac{1}{\mu(\theta)}u(x) \,, \quad u(x) \equiv \sum_{j,|q^j(x)|>1} |q^j(x)| \,.$$

The state dependent factor in the additional term of the cost function, $u(x)$, can be interpreted as an heuristic merit or penalty function that rewards multicolored columns for using fewer colors. This penalty function, and some possible variants, have the effect of softening the landscape, eroding sharp edges, such as in Figure 3b, into rounded hills and valleys, such as in Figure 3a. The actual functional form of this penalty function is inspired by the *tally function* used in the $P3$ heuristic of Hellerman and Rarick (1971) for sparse LU factorization. The temperature dependent parameter, $\mu(\theta)$, gives the inverse weight of the heuristic penalty function in the cost function $f(x, \mu)$.

Function $f(x, \mu)$ also has the following properties: (1) $f(x, 0) = f(x)$; (2) $f(x, \mu)$ is linear in $1/\mu$. Properties 1 and 2 suggest that we can cool the weight $1/\mu$ as we cool the temperature, much in the same way we control a parameter of the barrier functions in some constrained optimization algorithms, see McCormick (1983).

A possible implementation of this Heuristic Simulated Annealing, HSA, is as follows:

- Initialize parameters μ and θ, set a random partition, x, and initialize the auxiliary variables W, q, c, r, s, and the cost and penalty functions, f and h;

- For each proposed move, $x \to y$, compute the cost differentials

$$\delta_0 = f(y) - f(x) \text{ and } \delta_\mu = f(y, \mu) - f(x, \mu) .$$

- Accept the move with the Metropolis probability, $M(\delta_\mu, \theta)$. If the move is accepted, update x, W, q, c, r, s, f and h;

- After each batch of Metropolis sampling steps, perform a cooling step update

$$\theta \leftarrow (1 + \epsilon_1)\theta , \quad \mu \leftarrow (1 + \epsilon_2)\mu , \quad 0 < \epsilon_1 < \epsilon_2 << 1 .$$

Computational experiments show that the HSA successfully overcomes the difficulties undergone by the SSA, as shown in Stern (1991). As far as we know, this was the first time this kind of perturbative heuristic has been considered for SA. Pflug (1996) gives a detailed analysis for the convergence of such perturbed processes. These results are shortly reviewed is section H.1.

In the next section we are going to extend the idea of stochastic optimization to that of evolution of populations, following insights from biology. In zoology, there are many examples of heuristic merit or penalty functions, often called fitness or viability indicators, that are used as auxiliary objective functions in mate selection, see Miller (2000, 2001) and Zahavi (1975). The most famous example of such an indicator, the peacock's tail, was given by Charles Darwin himself, who stated: *"The sight of a feather in a peacock's tail, whenever I gaze at it, makes me feel sick!"* For Darwin, this case was an apparent counterexample to natural selection, since the large and beautiful feathers have no adaptive value for survival but are, quite on the contrary, a handicap to the peacock's camouflage and flying abilities. However, the theory presented in this section give us a key to unlock this mystery and understand the tale of the peacock's tail.

5.3 The Way of Sex: All for One

From the interpretation of the cooling constant given in the last section, it is clear that we would have a lower constant, resulting in a faster cooling schedule, if we used a richer set of single moves. Specially, if the additional moves could provide short-cuts in the configuration space, as the moves indicated by the dashed line in Figure 3a. This is one of the arguments that can be used to motivate another important class of stochastic evolution algorithms. Namely, Genetic Programming, the subject of the following sections. We will focus on a special class of problems known as functional trees. The general conclusions, however, remain valid in many other applications.

5.3.1   Functional Trees

In this section, we deal with methods of finding the correct specification of a complex function. This complex function must be composed recursively from a finite set, $OP = \{op_1, op_2, \ldots op_p\}$, of primitive functions or operators, and from a set, $A = \{a_1, a_2, \ldots\}$, of atoms. The k-th operator, op_k, takes a specific number, $r(k)$, of arguments, also known as the arity of op_k. We use three representations for (the value returned by) the operator op_k computed on the arguments $x_1, x_2, \ldots x_{r(k)}$:

$$op_k(x_1, \ldots x_{r(k)}) \quad , \qquad \begin{matrix} & op_k & \\ / & & \backslash \\ x_1 & \ldots & x_{r(k)} \end{matrix} \quad , \qquad \left(op_k\; x_1\; \ldots\; x_{r(k)}\right) \; .$$

The first is the usual form of representing a function in mathematics; the second is the tree representation, which displays the operator and their arguments as a tree; and the third is the prefix, preorder or LISP style representation, which is a compact form of the tree representation.

As a first problem, let us consider the specification of a Boolean function of q variables, $f(x_1, \ldots x_q)$, to mach a target table, $g(x_1, \ldots x_q)$, see Angeline (1996) and Banzhaf el al. (1998). The primitive set of operators and atoms for this problem are:

$$OP = \{\sim, \wedge, \vee, \rightarrow, \odot, \otimes\} \quad \text{and} \quad A = \{x_1, \ldots x_q, 0, 1\} \; .$$

Notice that while the first operator (not) is unary, the last five (and, or, imply, nand, xor) are binary.

x	y	$\sim x$	$x \wedge y$	$x \vee y$	$x \rightarrow y$	$x \odot y$	$x \otimes y$
0	0	1	0	0	1	1	0
0	1	1	0	1	1	0	1
1	0	0	0	1	0	0	1
1	1	0	1	1	1	0	0

The set, OP, of Boolean operators defined above is clearly redundant. Notice, for example, that

$$x_1 \rightarrow x_2 =\sim (x_1 \wedge \sim x_2) \; , \quad \sim x_1 = x_1 \odot x_1 \quad \text{and} \quad x_1 \wedge x_1 =\sim (x_1 \odot x_2) \; .$$

This redundancy may, nevertheless, facilitate the search for the best configuration in the problem's functional space.

Example 1a shows a target table, $g(a, b, c)$. As it is usual when the target function is an experimentally observed variable, the target function is *not* completely specified. Unspecified values in the target table are indicated by the don't-care symbol $*$. The two

solutions, f_1 and f_2, match the table in all specified cases. Solution f_1, however, is simpler and for that may be preferred, see section 4 for further comments.

a	b	c	g	f_1	f_2
0	0	0	1	1	1
0	0	1	1	1	1
0	1	0	*	1	0
0	1	1	*	1	0
1	0	0	0	0	0
1	0	1	1	1	1
1	1	0	0	0	0
1	1	1	1	1	1

```
        f1                                    f2
         |                                     |
         V                                     V
       /    \                            /           \
      ~      |                          ^             ^
      |      |                        /   \         /   \
      a      c                       ~     ~       |     |
                                     |     |       |     |
                                     a     b       a     c
```

$$f_1 = (\sim A) \vee C \ , \quad f_2 = (\sim A \wedge \sim B) \vee (A \wedge C) \ .$$

$$f_1 = (\vee (\sim A)\, C) \ , \quad f_2 = (\vee (\wedge (\sim A)\, (\sim B))\, (A \wedge C)) \ .$$

Example 1a: Two Boolean functional trees for the target $g(a, b, c)$.

As a second problem, let us consider the specification of a function for an integer numerical sequence, such as the Fibonacci sequence, presented in Koza (1983).

$$g(j) \equiv \begin{cases} j \ , & \text{if } j = 0 \vee j = 1 \ ; \\ g(j-1) + g(j-2) \ , & \text{if } j \geq 2 \ . \end{cases}$$

The following array, g^j, $0 \leq j \leq 20$, lists the first 21 elements of the Fibonacci sequence.

$$g = [0, 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, 233, 377, 610, 987, 1597, 2584, 4181, 6765] \ .$$

In this problem, the primitive set of operators and atoms are:

$$OP = \{+, -, \times, \sigma\} \ , \quad A = \{j, 0, 1\} \ ,$$

where j in an integer number, and the first three operators are the usual arithmetic operators. The specified function is used to compute the first $n + 1$ elements of the array f^j, seeking to mach the target array g^j, $0 \leq j \leq n$. The last primitive function is the recursive operator, $\sigma(i, d)$, that behaves as follows: When computing the j-th element, $f(j)$, $\sigma(i, d)$ returns the already computed element f^i, if i is in the range, $0 \leq i < j$, or a default value, d, if i is out of the range.

In the functional space of this problem, possible specifications for the Fibonacci function in prefix representation, are

$$(+\ (\sigma\ (-\ j\ 1)\ 1)\ (\sigma\ (-\ j\ (+\ 1\ 1)\ 0))) \ , \quad (+\ (\sigma\ (-\ j\ 1)\ 1)\ (+\ 0\ (\sigma\ (-\ j\ (+\ 1\ 1)\ 0)))) \ .$$

Example 2a: Two functional trees for the Fibonacci sequence.

Since the two expressions above are functionally equivalent, the first one may be preferable for being simpler, see section 4 for further comments.

As a third problem, we mention Polynomial Network models. These functional trees use as primitive operators linear, quadratic or cubic polynomials in one, two or three variables. For several examples and algorithmic details, see Farlow (1984), Madala and Ivakhnenko (1994) and Nikolaev and Iba (2006). Figure 4 shows a simple network used for sales forcast, a detailed report is given in Lauretto et al. (1995). Variable x_5 is a magazine's sales forecast obtained by a VARMA time series model using historic sales, econometric and calendric data. Variables x_1 to x_4 are qualitative variables (in the scale: Bad, Weak, Average, God, Excellent) to assess the appeal or attractiveness of an individual issues of the magazine, namely: (1) cover impact; (2) editorial content; (3) promotional items; and (4) point of sale marketing.
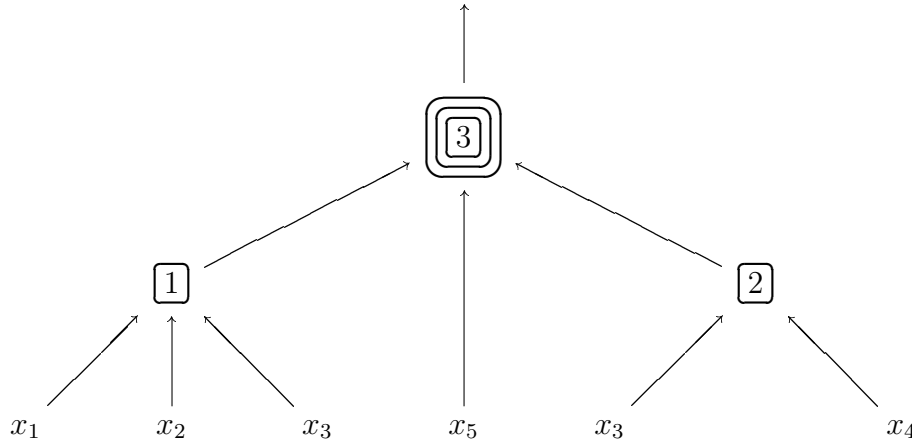
Figure 4: Polynomial Network.
Rings on a node: 1- Linear; 2- (incomplete) Quadratic; 3- (incomplete) Cubic.

Of course, the optimization of a Polynomial Network is far more complex than the optimization of Boolean or algebraic etworks, since not only topology has to be optimized (identification problem), but also, given a topology, the parameters of the polynomial function have to be optimaized (estimation problem). Parameter optimization of sub-trees can be based on Tikhonov regularization, ridge regression, steepest descent or Partan gradient rules. For several examples and algorithmic details, see Farlow (1984), Madala and Ivakhnenko (1994), Nikolaev and Iba (2001, 2003, 2006), and Stern (2008).

5.3.2 Genetic Programming

Starting from a given random tree, one can start an SA type search in the problem's (topological) space. In GP terminology, the individual's functional specification is called its *genotype.* the individual's expressed behavior, or computed solutions, is called its *phenotype.* Changing a genotype to a neighboring one is called a *mutation.* The quality of a phenotype, its performance, merit or adaptation, is measured by a *fitness* function.

While SA looks at the evolution of a single individual, GP looks at the evolution of a population. A time parameter, t, indexes the successive generations of the evolving population. In GP, individuals typically have short lives, surviving only a few generations before dying. Meanwhile, populations may evolve for a very long time.

In GP an individual may, during its ephemeral life, share information, that is, swap (copies) of its (partial) genome, with other individuals. This genomic sharing process is called *sex.* In GP an individual, called a *parent*, may also participate in the creation of a new individual, called its *child*, in a process called *reproduction.* In the reproduction process, an individual gives (partial) copies of its genotype to its offspring. Reproduction involving only one parent is called asexual, otherwise it is called a sexual reproduction.

In the following list, a set of possible mutation and sex operators are given:

1- Point leaf mutation: Replace a leaf atom by an other atom.

2- Point operator mutation: Replace a node operator by a compatible operator.

3- Shrink mutation: Replace a sub-tree by a leaf with a single atom.

4- Grow mutation: Replace the atom at a leaf by a random tree.

5- Permutation: Change the order of the children of a given node.

6- Gene duplication: Replace a leaf by a copy of a sub-tree.

7- Gene inversion: Switch two sub-trees.

8- Crossover: Share or exchange sub-trees between individuals.

The first five operators, involving only one sub-tree, are sometimes called (proper) mutations, while the last three operators, involving two or more separate sub-trees, are called recombinations. Also notice that the first seven operators involve only one individual, while crossover involves two or more. This list of mutation and recombination operators is redundant but, again, this redundancy may also facilitate the search for the best configuration in the problem's functional space.

We should mention that the terms used to name these operators are not standard in the field of GP, and even less so in biology, genetics, zoology and botany. We should also mention that the forms of GP presented in this section, do not explore the possibility of allowing individuals to carry a (redundant) set of two or more homologous (similar

but not identical) specifications (genes), a phenomenon known as diploidy or multiploidy. Diploidy is common in eukaryotic (biological) life, and can provide a much richer structure and better performance to GP.

Sexual reproduction can be performed by crossover, with parents giving (partial) copies of their genome to the children. The following examples show a pair of parents and children generated by a single crossover, for some of the problems considered in the last section. A square parenthesis in the prefix representation indicates a crossover point. The tree representation would indicate the same crossover points by broken edges (=). Notice that in these examples the is a child corresponding to a solution presented in the last section.

```
        f1                  f2                              f3
        |                   |                               |
        V                   V                               V
      /    \              /    =                          /    \
     ∧       =           |       ∧        ⇒              ∧         ∧
    /  \     |    |       b      /  \              /  \      /  \      /  \
   ~    ~    a              |    |            ~    ~    |    |
   |    |                   |    |            |    |    |    |
   a    b                   a    c            a    b    a    c
```
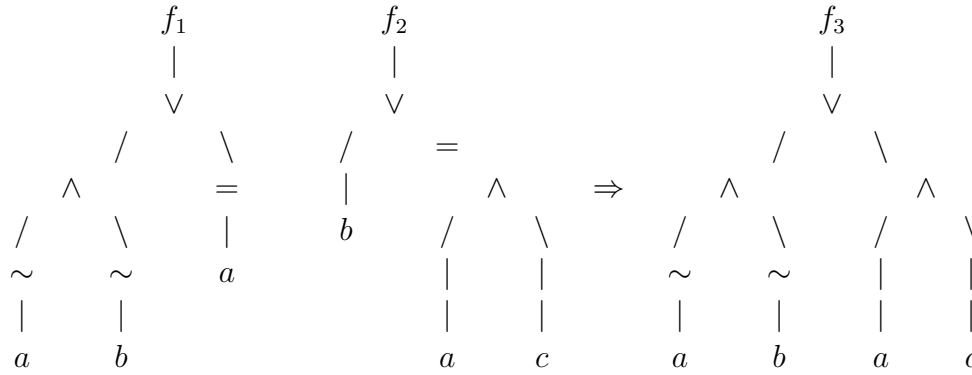
Example 1b: Crossover between Boolean functional trees.

Parents: $(* [\sigma (- j\ 1)\ 1]\ (*\ j\ j))$, $(+ (\sigma (- j\ (+\ 1\ 1)\ 0))\ [- j\ 1]\ )$;

Children: $(* [- j\ 1]\ (*\ j\ j))$, $(+ (\sigma (- j\ (+\ 1\ 1)\ 0))\ [\sigma (- j\ 1)\ 1]\ )$.

Example 2b: Crossover between arithmetic functional trees.

Finally, the reproduction and survival selection processes in GP assume that individuals are chosen from the general population according to sampling probabilities called the *mating* (or representation) distribution and the *survival* distribution, respectively. Some general policies used to specify these probability distributions, based on the individual's fitness, are given below:

1- Top Rank Selection: The highest ranking (best fit) individual is selected.

2- High Pressure Selection: An individual is selected from the population with a probability that increases sharply (super-linearly) with its fitness or fitness' rank.

3- Fitness Proportional Selection: An individual is selected from the population with a probability that is proportional to its fitness.

4- Rank Proportional Selection: An individual is selected from the population with a probability that is proportional to its fitness' rank.

5- Low Pressure Selection: An individual is selected from the population with a probability that increases modestly (sub-linearly) with its fitness or fitness' rank.

6- Tournament Selection: A small subset is sampled at random (uniformly) from the population, from which the best (one or two) individuals are selected.

7- Uniform Selection: An individual is selected from the population with uniform probability.

These processes are supposed to mimic biological selection mechanisms, including sexual differentiation, like male and female (alleged) behavior, familiar and other sub-population structures, etc.

5.3.3   Schemata and Parallelism

A possible motivation for developing populational evolutionary algorithms like GP, instead of single individual evolutionary algorithms, like straight SA, is to consider a richer and better neighborhood structure. The additional moves made available should provide short-cuts in the problem's configuration space, lowering the cooling constant and allowing a faster convergence of the algorithm.

The *intrinsic parallelism* argument, first presented in Holland (1975), proves that, under appropriate conditions, GP is likely to succeed in providing such a rich neighborhood structure. The mathematical analysis of this argument is presented in section H.2, see also Reeves (1993, Ch.4 Genetic Algorithms). According to Reeves,

> *"The underlying concept Holland used to develop a theoretical analysis of his GA [GP] was that of* schema*. The word comes from the past tense of the Greek verb* $\epsilon\chi\omega$, echo, *to have, whence it came to mean shape or form; its plural is* schemata*."* (p.154)

Schemata are partially specified patterns in a program, like partially specified segments of prefix expressions, or partial code for functional sub-trees. The *length* and *order* of a schema are the *distance* between the first and last defined position on the schema, and the number of defined positions, respectively, see section H.2. The Intrinsic Parallelism theorem states that the number of schemata (of order l and length $2l$, in binary coded programs, in individuals of size n) present in a population of size m, is proportional m^3. The crossover operator enriches the neighborhood of an individual with the schemata present in other individuals of the population. If, as suggested by the implicit parallelism theorem, the number of such schemata is large, GP is likely to be an effective strategy.

Schaffer (1987, p.89), celebrates this theorem stating that:

> *"this [intrinsic parallelism] constitutes the only known example of combinatorial explosion working to advantage instead of disadvantage."*

Indeed, Schaffer has ample reason to praise Holland's result. Nevertheless, we must analyze this important theorem carefully, in order to understand its consequences correctly. In particular, we should pay close attention to the unit, u, used to measure the population size, m. As shown in detail in section H.2, this unit, $u = 2^l$, is itself exponential in the schemata order. Therefore, the combinatorial explosion works to our advantage as long as we use short schemata, relative to the log-size of the population. This situation is described by Reeves as:

> *"Thus the ideal situation for a GA [GP] are those where short, low-order schemata combine with each other to form better and better solutions. The assumption that this will work is called by Goldberg (1989) the* building-block hypothesis*. Empirical evidence is strong that this is a reasonable assumption in many problems."* (p.158)

One key question we must face in order to design a successful GP application is, therefore: How then can we organize our working space so that our programming effort can rely on short schemata?

The solution to this question is well known to computer scientists and software engineers: Organize the programs hierarchically (recursively) as self-contained (encapsulated) building-blocks (modules, functions, objects, sub-routines, etc.). The next section is dedicated to the study of modular organization, and its spontaneous emergence in complex systems.

5.4   Simple Life: Small is Beautiful

The biological world is an endless source of inspiration for improvements and variations in GP (of course, one should also be careful not to be carried away by superficial analogies). A nice anthology of introductory articles can be found in the book by Michod and Levin (1988), *The Evolution of Sex: An Examination of Current Ideas.* Let us begin this section with an interesting biological example.

It is a well known phenomenon that bacteria can develop antibiotic resistance. Among the most common mechanisms conferring resistance to new antibiotics, one can list: Agents that modify or destroy the antibiotic molecular structure; Agents that modify or protect the antibiotic targets; New pathways offering alternatives to those blocked by the antibiotic action; etc. However, all these mechanisms entail a fitness cost to the modified individuals. At the very least, there is the cost of complexity, that is, the cost of building and maintaining these new mechanisms. Hence, if the selective pressure of the antibiotic presence is interrupted, resistant bacterial populations will often revert to non-resistant, see for example Björkholm et al. (2001).

This biological example can be interpreted as the embodiment of *Okcam's razor* or *lex parsimoniae*, an epistemological principle stated by the 14th-century English logician friar William of Ockham, in the following forms:

  - *Entia non sunt multiplicanda praeter necessitate,* or

  - *Pluralitas non est ponenda sine neccesitate.*

that is, entities should not be created or multiplied without necessity.

In section 4.1 we will see how well this principle applies to statistical models, and how it can be enforced. In section 4.2 we will examine *introns*, a phenomenon that at first glance appears to contradict Okcam's razor. Nevertheless, we will also see how introns allow building blocks to appear spontaneously as an emergent feature in GP.

5.4.1 Overfitting and Regularization

This section discusses the use of Okcam's razor in statistical modeling. As an illustrative example, we use a standard normal multiple linear regression model. This model states that $y = X\beta + u$, X $n \times k$, where n is the number of observations, k is the number of independent variables, $\beta \in]-\infty, \infty[^k$ is the vector of regression coefficients, and u is a Gaussian white noise such that $E(u) = 0$ and $\mathrm{Cov}(u) = \sigma^2 I$, $\sigma \in [0, \infty[$, see DeGroot (1970), Hocking (1985) and Zellner (1971). Using the standard diffuse prior $p(\beta, \sigma) = 1/\sigma$, the joint posterior probability density, $f(\beta, \sigma \,|\, y, X)$, and the MAP (maximum a posteriori) estimators for the parameters are given by:

$$
\begin{aligned}
f(\beta, \sigma \,|\, y, X) &= \frac{1}{\sigma^{n+1}} \exp\left(-\frac{1}{2\sigma^2}\left((n-k)s^2 + (\beta - \hat{\beta})'X'X(\beta - \hat{\beta}) \right)\right), \\
\hat{\beta} &= (X'X)^{-1}X'y, \\
\hat{y} &= X\hat{\beta}, \\
s^2 &= (y - \hat{y})'(y - \hat{y})/(n-k).
\end{aligned}
$$

In the polynomial multiple linear regression model of order k, the dependent variable y is explained by the powers 0 through k of the independent variable x, i.e., the regression matrix element at row i and column j is $X_i^j = (x_i)^{j-1}$, $i = 1 \ldots n$, $j = 1 \ldots k+1$. Note that the model of order k has dimension $d = k + 2$, with parameters $\beta_0, \beta_1, \ldots \beta_k$, and σ.

In the classical example presented in Sakamoto et al. (1986, ch.8), we want to fit a linear regression polynomial model of order k,

$$
y = \beta_0 \mathbf{1} + \beta_1 x + \beta_2 x^2 \ldots + \beta_k x^k + N(0, \sigma I)
$$

through the $n = 21$ points, (x_i, y_i), in Table 1.

i	x_i	y_i	i	x_i	y_i	i	x_i	y_i
1	0.00	0.125	8	0.35	-0.135	15	0.70	0.035
2	0.05	0.156	9	0.40	0.105	16	0.75	0.327
3	0.10	0.193	10	0.45	0.131	17	0.80	0.061
4	0.15	-0.032	11	0.50	0.154	18	0.85	0.383
5	0.20	-0.075	12	0.55	0.114	19	0.90	0.357
6	0.25	-0.064	13	0.60	-0.094	20	0.95	0.605
7	0.30	0.006	14	0.65	0.215	21	1.00	0.499

Table 5.1: Sakamoto's data set for polynomial model

This example was produced by Sakamoto simulating the i.i.d. stochastic process

$$y_i = g(x_i) + 0.1 * N(0,1) , \quad g(x) = \exp((x - 0.3)^2) - 1 ,$$

where the target function, $g(x)$, cannot be expressed exactly as a finite order linear regression polynomial model.

Figure 5 presents the target function in the example's range, the data set (Sakamoto's set in 5a and a second set generated by the same stochastic process in 5b), and the regression polynomials of orders 0 through 5. In this example, all the available data points are used to fit the model. An alternative procedure would be to divide the available data in two sets, the *training set*, used to adjust the model, and the *test set*, used to test the model's predictive or extrapolation power.

Just by visual inspection, one can come to the following conclusions:

- If the model is too simple, it fails to capture important information available in the data, making poor predictions.

- If the model is too complex, it *overfits* the training data, that is, the curve $f(t)$ tends to become an interpolation curve, but the curve becomes unstable and predicted values become meaningless.

The polynomial regression model family presented in the example is typical, in the sense that it offers a class o models of increasing dimension, or complexity. This poses a *model selection* problem, that is, deciding, among all models in the family, the "best" adapted to the data. It is natural to look for a model that accomplishes a small empirical error, the estimated model error in the training data, R_{emp}. A regression model is estimated by minimizing the 2-norm empirical error. However, we cannot select the "best" model based only on the empirical error, because we would usually select a model of very high complexity. In general, when the dimensionality of the model is high enough, the empirical error can be made equal to zero by simple interpolation. It is a well known fact in statistics (or learning theory), that the prediction (or generalization) power of such high dimension models is poor. Therefore the selection criterion has to penalize also the
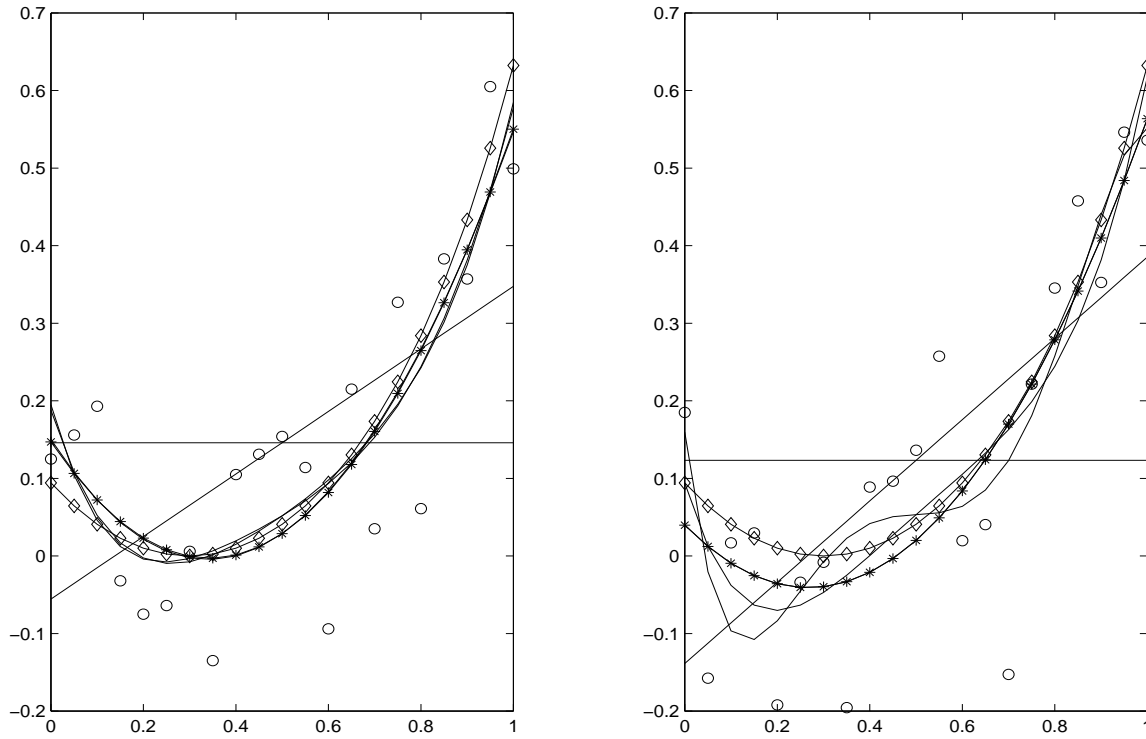
Figure 5a,b: Target function, data points, and polynomial regressions of order 0 to 5;
○: Data points; ⋄: Target function; ∗: Best (quadratic) polynomial regression.

model dimension. This is known as a *regularization* mechanism.

Some model selection criteria define $R_{pen} = r(d, n)R_{emp}$ as a penalized (or regularized) error, using a regularization factor, $r(d, n)$, where d is the model dimension and n the number of training data points. Common regularization factors, using $p = (d/n)$, are:

- Akaike's final prediction error: $\text{FPE} = (1 + p)/(1 - p)$,

- Schartz' Bayesian criterion: $\text{SBC} = 1 + \ln(n)p/(2 - 2p)$,

- Generalized cross validation: $\text{GCV} = (1 - p)^{-2}$,

- Shibata model selector: $\text{SMS} = 1 + 2p$,

All these regularization factors are supported by theoretical arguments as well as by empirical performance; other common regularization methods are Akaike information criterion

(AIC), and Vapnik-Chervonenkis (VC) prediction error. For more details, see Akaike (1970 and 1974), Barron (1984), Breiman (1984), Cherkassky (1998), Craven (1979), Michie (1994), Mueller (1994), Shibata (1981), Swartz (1978), Unger (1981) and Vapnik (1995, 1998).

We can also use the FBST as a model selection criterion by testing the hypothesis of some of its parameters being null, as detailed in Pereira and Stern (2001). The FBST version of Okcam's razor states:

- *Do not include in the model a new parameter unless there is strong evidence that it is not null.*

Table 2 presents the empirical error, EMP $= ||y - \hat{y}||_2^2/n$, for models of order k ranging from 0 to 5, several regularization criteria previously mentioned as well as the Akaike information criterion (AIC), as computed by Sakamoto. Table 2 also presents the e-value supporting the hypothesis $H : \beta_k = 0$, that is, the hypothesis stating that the model is in fact of order $k - 1$.

Order	EMP	FPE	SBC	GCV	SMS	AIC	FBST
0	0.03712	0.04494	0.04307	0.04535	0.04419	-07.25	0.00
1	0.02223	0.02964	0.02787	0.03025	0.02858	-20.35	0.00
2	0.01130	0.01661	0.01534	0.01724	0.01560	-32.13	0.00
3	0.01129	0.01835	0.01667	0.01946	0.01667	-30.80	1.00
4	0.01088	0.01959	0.01751	0.02133	0.01710	-29.79	0.99
5	0.01087	0.02173	0.01913	0.02445	0.01811	-27.86	1.00

Table 5.2: Selection Criteria for the Polynomial Model

Alternative approaches to regularization are given by Jorma Rissanen's MDL (minimum description length) and Chris Wallace's MML (minimum message length). Following an old idea of Andrey Kolmogorov, these criteria make direct use of a program's code-length as a measure of complexity, see Rissanen (1978, 1989), Wallace and Boulton (1968) and Wallace and Dowe (1999).

5.4.2 Building Blocks and Modularity

As seen in section 3, GP can produce polynomial networks that are very similar to the polynomial regression models presented in the last section. The main difference between the polynomial networks and the regression models lies in their generation process: While the regression models are computed by a deterministic algorithm, the GP networks are generated by a random evolutionary search. However, if one uses compatible measures of performance for the GP fitness function and the regression (penalized or regularized)

error, one could expect GP to produce networks that somehow fulfill Okcam's parsimony principle.

Surprisingly, this is not so. P. Angeline (1994, 1996) noted that GP generated networks typically contain large segments of *extraneous* code, that is, code segments that, if removed, do not (significantly) alter the solution computed by the network. Trivial examples of extraneous code segments are $(+ \; s \; 0)$ and $(* \; s \; 1)$, where s is a sub-expression. By their very definition, extraneous code segments cannot (significantly) contribute to an individual's fitness, and hence to its survival or mating probabilities. However, Angeline noticed that the presence of extraneous code could significantly contribute to the expected fitness of the individual's descendents! Apparently, the role of these (sometimes very large) patches of inert code is to isolate important blocks of working code, and to protect these blocks from being broken at recombination (destructive crossover).

In biological organisms, the genetic code of eukaryots exhibits similar regions of code (DNA) that are or are not expressed in protein synthesis; these regions are called *exons* and *introns*, respectively. Introns do not directly code amino-acid sequences in proteins, nevertheless, they seem to have an important role in the meta-control of the genetic material expression and reproduction.

Subsequent work of several authors tried to incorporate meta-control parameters to GP. Iba and Sato (1993, p.548), for example, propose a meta-level strategy for GP based on a self-referential representation, where

> *"[a] self-referential representation maintains a meta-description, or meta-prescription, for crossover. This meta-genetic descriptions are allowed to co-evolve with the gene pool. Hence, genetic and meta-genetic code variations are jointly selected. How well the genetic code is adapted to the environment is translated by the merit or objective function which, in turn, is used for the immediate, short-term or individual selection process. How well the genetic and meta-genetic code are adapted to each other impacts on the system's evolvability, a characteristic of paramount importance in long-run survival of the species."*

Functional trees, for example, can incorporate edge annotations, like probability weights, linkage compatibility or affinity, etc. Such annotations are meta-parameters used to control the recombination of the sub-tree directly bellow a given edge. For example, weights may be used to specify the probability that a recombination takes place at that edge, while linkage compatibility or affinity tags may be used to identify homologous or compatible genes, specifying the possibility or probability of swapping two sub-trees. Other annotations, like context labels, variable type, etc., may provide additional information about the possibility or probability of recombination or crossover, the need of type-cast operations, etc. When such metacontrol annotations coevolve in the stochastic optimization process,

they may be interpreted as a spontaneously emergent semantics. Any semantic information may, in turn, be used in the design of acceleration procedures based on heuristic merit functions, like the example studied in section 5.2.3.

Banzahf (1998, ch.6, p.164), gives a simple example of functional tree annotation:

> *"Recently, we introduced the explicitly defined introns (EDI) into GP. An integer value is stored between every two nodes in the GP individual. This integer value is referred as the EDI value (EDIV). The crossover operator is changed so that the probability that crossover occurs between any two nodes in the GP program is proportional to the integer value between the nodes. That is, the EDIV integer value strongly influences the crossover sites chosen by the modified GP algorithm, Nordin et al. (1996).*
>
> *The idea behind EDIVs was to allow the EDIV vector to evolve during the GP run to identify the building blocks in the individual as an emergent phenomenon. Nature may have managed to identify genes and to protect them against crossover in a similar manner. Perhaps if we gave the GP algorithm the tools to do the same thing, GP, too, would learn how to identify and protect the building blocks. If so, we would predict that the EDIV values within a good building block should become low and, outside the good block, high."*

Let us finish this section presenting two interpretations for the role of modularity in genetic evolutionary processes. This interpretations are common in biology, computer science and engineering, an indication that they provide powerful insights. These two metaphors are commonly referred to as:

- New *technology dissemination* or *component design substitution*, and

- *Damage control* or *repair mechanism.*

The first interpretation is perhaps the more evident. In a modular system, a new design for an old component can be easily incorporated and, if successful, be rapidly disseminated. A classical example is the replacement of mechanical carburetors by electronic injection as the standard technology for this component of gasoline engines in the automotive industry. The large assortment of *upgrade kits* available in any automotive or computer store gives a strong evidence of how much these industries rely on modular design. The second interpretation explains the possibility for the "continued evolution of germlines otherwise destined to extinction", see Michod and Levin (1988). A classic illustration related to the damage control and repair mechanisms offered by modular organization is given by the Hora and Tempus parable of Simon (1996), presented in section 6.4.

The lessons learned in this section may be captured by the following dicta of Herbert Simon:

> *"The time required for the evolution of a complex form from simple ele-*

> *ments depends critically on the number and distribution of potential interme-diate stable subassemblies."* Simon (1996, p.190).

> *"Hierarchy, I shall argue, is one of the central structural schemes that the architect of complexity uses."* Simon (1996, p.184).

5.5 Evolution of Theories

The last sections presented a general framework for the stochastic evolution of complex systems. Figure 6 presents a systemic diagram of biological production, according to this framework. This diagram, is also compatible with the current biological theories of life evolution, provided it is considered as a schematic simplification focusing on our particular interests.

The comparison of this biological production diagram with the scientific production diagram presented in section 1.5. motivates several analogies which may receive further encouragement from a comment by Davis and Steenstrup (1987, p.2):

> *"The metaphor underlying genetic algorithms is that of natural evolution. In evolution, the problem each species faces is one of searching for beneficial adaptations to a complicated and changing environment. The 'knowledge' that each species has gained is embodied in the makeup of the chromosomes of its members."*

According to this view, computational (or biological genetic) programs are perceived as coded knowledge acquired by a population. An immediate generalization of this idea is to consider the evolution of other corpora of knowledge, embodied in a variety of media. Our main interest, given the scope of this book, is in the evolution of scientific theories and their supporting statistical models. This is the topic discussed in this and the next sections. For some very interesting qualitative analyses related to this subject see Richards (1989, appendix II) and Lakatos (1978a,b).

Section 5.1 considers several ways in which statistical models can be nested, mixed and separated. It also analyzes the series-parallel composition of several simpler and (nearly) independent models. Section 5.2 is devoted to complementary models. Complementarity is a basic form of model composition in quantum mechanics that has received, so far, little attention in other application areas. All these forms of model transformation and combination should provide a basic set of mutations and recombination operators in an abstract modeling space. In this section we focus on the statistical operations themselves, leaving some of the required epistemological analyses and historical comments to sections 6 and 7.

Somatic behavior				Genetic code
Individual ontogenesis	$\Leftarrow$	Epigenetic development	$\Leftarrow$	Individual genotypes
$\Downarrow$				$\Uparrow$
Fittest survival		Live/Dead organism		Genetic Mutation
$\Downarrow$				$\Uparrow$
Mating competition	$\Rightarrow$	Reproductive representation	$\Rightarrow$	Sexual recombination
Phenotypic space				Genotypic space
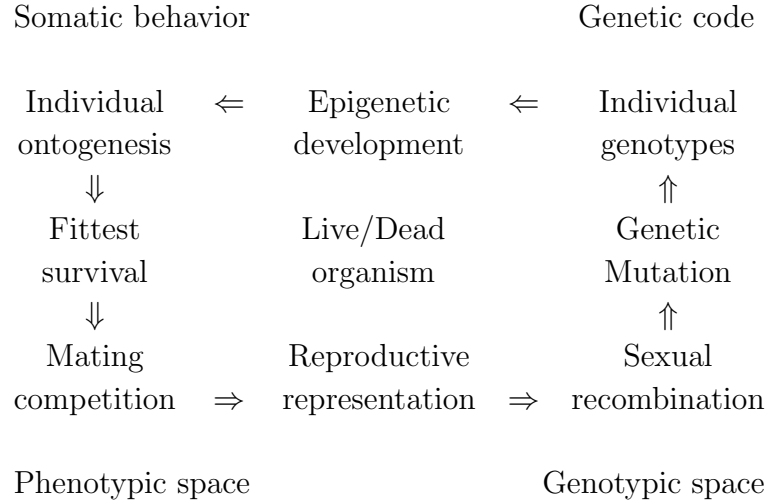
Figure 6: Biological production diagram.

5.5.1   Nested, Mixture, Separate and Series-Parallel Models

In this subsection we use some examples involving the (two-parameter) Weibull (W2) and Gompertz (G2) probability models. The hazard (or failure rate) functions, h_{W2} and h_{G2}, the reliability (or survival) function, r_{W2} and r_{G2}, and the density function, f_{W2} and f_{G2}, of these models are given by:

$$h_{W2}(x \mid \beta, \gamma) = \frac{\beta}{\gamma^{\beta}} x^{\beta-1} \ ; \ \ r_{W2} = \exp\left(-\left(\frac{x}{\gamma}\right)^{\beta}\right) \ ; \ \ f_{W2} = \frac{\beta}{\gamma^{\beta}} x^{\beta-1} \exp\left(-\left(\frac{x}{\gamma}\right)^{\beta}\right) \ ;$$

$$h_{G2}(x \mid \alpha, \lambda) = \lambda \alpha^{x} \ ; \ \ r_{G2} = \exp\left(\frac{-\lambda}{\log \alpha}\left(\alpha^{x}-1\right)\right) \ ; \ \ \text{and} \ \ f_{G2} = \lambda \alpha^{x} \exp\left(\frac{-\lambda}{\log \alpha}\left(\alpha^{x}-1\right)\right) \ .$$

The parameters: β and γ for the Weibull model; and λ and α for the Gompertz model, are known, respectively, as the scale and shape parameters. Notice that $h = f/r$, and $r = 1 - F$, that is, the reliability function is the complement of the cumulative distribution function F.

These probability models are used in reliability theory to study the characteristics of the survival (or life) time of a system, until it first fails (or dies). It can be shown, see Barlow and Prochan (1981), Gavrilov (1991, 2001) and appendix H.3, that the Weibull distribution is adequate to describe the survival time of many allopoietic, manufactured or industrial systems, while the Gompertz distribution is adequate to describe the life time of many autopoietic, biological or organic systems. In this setting, the key difference between autopoietic and allopoietic systems is the nature of their ontogenesis or assembling process, as described in the next paragraphs. Reasonable assumptions concerning the systems' ontogenesis will render either the Weibull or the Gompertz distributions as asymptotic eigen-solutions.

The assemblage of allopoietic systems is assumed to be subject to rigid protocols of quality control, to assure that parts and components as well as the final product, work properly. The good quality of the parts and components allows the use of efficient projects and streamlined designs, with little redundancy and practically no waste. Project optimization provides the designer of such products the means to minimize the use of space, material resources, and even assembling time. The lack of redundancy, however, implies that the failure of just a few or even only one small component can disable the system.

In contrast, an autopoietic system is assumed to be self-assembled. The very nature of organic ontogenesis does not allow for strict quality control. For example, in embryonic or fetal development there is not an opportunity to check individual cells, nor is there a mechanism for replacing defective ones. The viability of autopoietic systems relies not on quality control of individual components, but on massive redundancy and parallelism.

Let us now examine more closely some of the details of these statistical models. In so doing we will also be able to explain several modes of model composition.

In the Weibull model, the scale parameter, γ, is approximately the 63rd lifetime percentile, regardless of the value of the shape parameter. By altering its shape parameter, β, the (two-parameter) Weibull distribution can take a variety of forms, see Figure 7 and Dodson(1994). Some particular values of the shape parameter are important special cases: for $\beta = 1$, it is the exponential distribution; for $\beta = 2$, it is the Rayleigh distribution; for $\beta = 2.5$, it approximates the lognormal distribution; for $\beta = 3.6$, it approximates the normal distribution; and for $\beta = 5.0$, it approximates the peaked normal distribution. The flexibility of the Weibull distribution makes it very useful for empirical modeling, specially in quality control and reliability. The regions $\beta < 1$, $\beta = 1$, and $\beta > 1$ correspond to decreasing, constant and increasing hazard rates. These three regions are also known as infant mortality, memoryless, and wearout. In the limit case $\beta = 1$, the Weibull degenerates into the Exponential distribution. This (no) aging regime represents a simple element with no structure exhibiting, therefore, the memoryless property of constant failure rate, $h_E(x \,|\, \gamma) = 1/\gamma$.

The affine transformation $x = x' + \alpha$ leads to the (three parameter) Truncated Weibull distribution. A location (or threshold) parameter, $\alpha > 0$ represents beginning observation of a Truncated Weibull variate at $t = 0$, after it has already survived the period $[-\alpha, 0[$. For the sake of comparison, the reliability functions of the (one-parameter) Exponential, and the two and three-parameter Weibull distributions are given next;

$$r_E(x \,|\, \gamma) = \exp\left(-\left(\frac{x}{\gamma}\right)\right) \;\; ; \;\; r_{W2}(x \,|\, \beta, \gamma) = \exp\left(-\left(\frac{x}{\gamma}\right)^\beta\right) \; ;$$

$$r_{W3}(x \,|\, \alpha, \beta, \gamma) = \frac{1}{r_{W2}(\alpha \,|\, \beta, \gamma)} \exp\left(-\left(\frac{x + \alpha}{\gamma}\right)^\beta\right) \; .$$
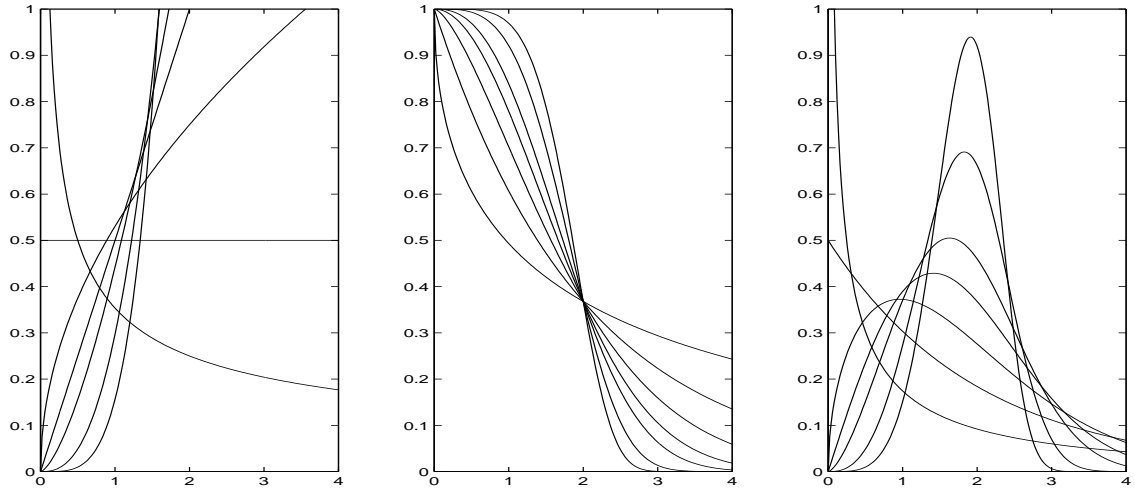
Figure 7: Shapes of the Weibull Distribution, h, r and f.
Parameters: $\gamma = 1$, $\beta = 0.5, 1.0, 1.5, 2.0, 2.5, 3.6, 5.0$.

In the example at hand we have three *nested models*, in which a distribution with less parameters (or degrees of freedom) is a special case (a sub-manifold in the parameter space) of a distribution with more parameters (or degrees of freedom): The (one-parameter) Exponential distribution is a special case of the (two-parameter) Weibull distribution which, in turn, is a special case of the (three-parameter) Truncated Weibull distribution. Nesting is one of the basic modes of relating different statistical models. For examples of the FBST used for model selection in nested models see Ironi at al. (2002), Lauretto et al. (2003), Stern and Zacks (2002).

The (two-parameter) Weibull distribution has also an important theoretical property: Its functional form is invariant by serial composition. If n i.i.d. random variables have Weibull distribution, $X_i \sim f(x \mid \beta, \gamma)$, then the first failure is a Weibull variate with characteristic life $\gamma/n^{1/\beta}$, i.e. $X_{[1,n]} \sim f(x \mid \beta, \gamma/n^{1/\beta})$. This is a key property for its characterization as a stable distribution, that is, for the characterization of the Weibull distribution as an (asymptotic) eigensolution. For applications in the context of extreme value theory, see Barlow and Prochan (1981).

While a series system fails when its first element fails, a parallel system fails when its last element fails. Figure 8 gives the standard graphical representation of series and parallel systems. This representation is inspired in circuit theory: While in a serial system the current flow is cut if a single element is cut, in a parallel system the current flow is cut only if all elements are cut. Series / parallel composition are the two basic modes used in Reliability Engineering for structuring and analyzing complex systems. Some of the statistical properties of these structures are captured in the form of algebraic lattices, see Barlow and Prochan (1981) and Kaufmann et al. (1977). Some of these properties

are similar or analog to the compositional rules analyzed in section A.4 and Borges and Stern (2007). The characterization of the Gompertz as a limit distribution for parallel systems is given in appendix H.3, following Gavrilov (1991).
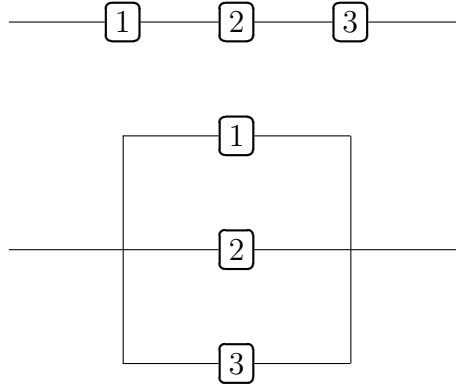
Figure 8: Series and Parallel Systems.

Imagine a situation in which a scientist receives a data bank of observed individual lifetimes in a population. The scientist also knows that all individuals in the population are of the same nature, that is, the population is either entirely allopoietic, H_1, or autopoietic, H_2. Since hypotheses H_1 and H_2 imply life distributions with distinct functional forms, the scientist could use his/her observed life data to decide which hypothesis is correct (or more adequate). This situation is known in statistics as the problem of *separate hypotheses*. The scientist could also be faced with a mixed population, a situation in with a fraction w_1 of the individuals are allopoietic, and a fraction w_2 of the individuals are autopoietic. In this situation the scientist could use his/her observed data to infer the fractions or *weights*, w_1 and w_2, in the *mixture model*.

For mixture models in the general, the p.d.f. of the data is a convex linear combination of fixed candidate densities. Writting the model's vector parameter as $\theta = [w, \psi_1, \ldots \psi_m]$,

$$ f(x \mid \theta) = w_1 f_1(x \mid \psi_1) + \ldots + w_m f_m(x \mid \psi_m) \ , \quad w \geq 0 \mid w\mathbf{1} = 1 \ , $$

and the model's likelihood function is

$$ f(X \mid \theta) = \prod\nolimits_{j=1}^{n} \sum\nolimits_{k=1}^{m} w_k f_k(x_j \mid \psi_k) \ . $$
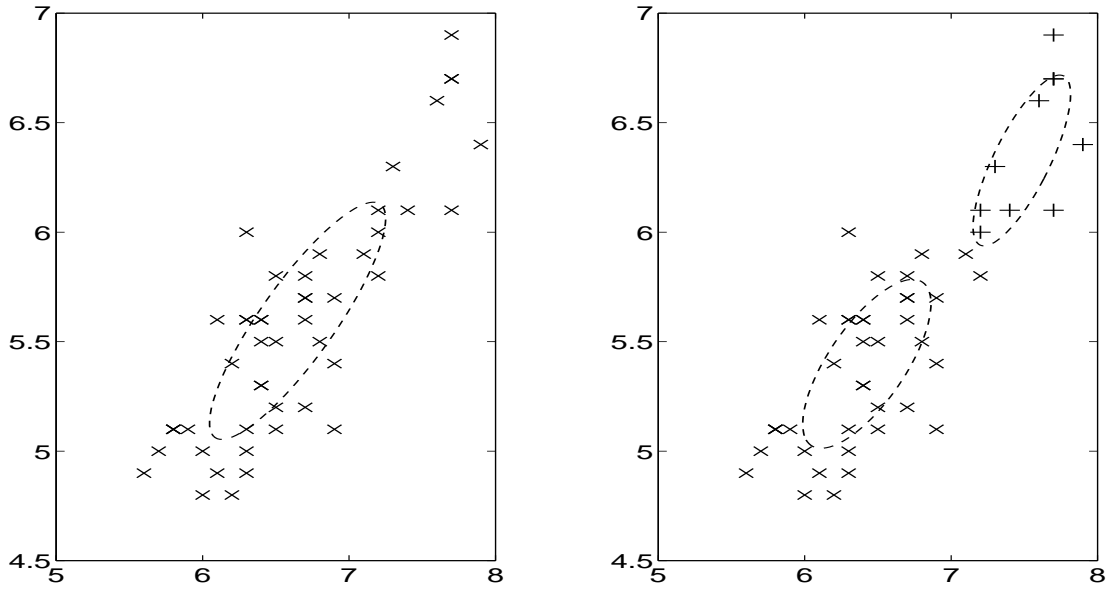
Figure 9a,b: Mixture models with 1 and 2 bivariate-Normal components.

In mixture analysis for unsupervised classification, we assume that the data comes from two or more subpopulations (classes), distributed under distinct densities. Statistical mixture models may also be able to infer the classification probabilities for each data point, see Figure 9. In a *heterogeneous mixture* model, the components in the mixture have distinct functional forms. In a *homogeneous mixture* model, all components in the mixture have the same functional form. For several applications of these models, see Fraley (1999), Lauretto et al. (2006, 2007), Robert (1996) and Stephens (1997).

5.5.2   Complementary Models

According to Bohr, the word *Complementarity* is used

> *"...to characterize the relationship between experiences obtained by different experimental arrangements and visualizable only by mutually exclusive ideas...".* (N.Bohr II, Natural Philosophy and Human Cultures, p.30)
> *"Information regarding the behavior of an object obtained under definite experimental conditions may, however, ...be adequately characterized as complementary to any information about the same object obtained by some other experimental arrangement excluding the fulfillment of the first conditions. Although such kinds of information cannot be combined into a single picture by means of ordinary concepts, they represent indeed equally essential aspects of*

any knowledge of the object in question which can be obtained in this domain."
(Bohr 1938, p.26).

In quantum Mechanics, at least from a historical perspective, the most important complementarity relations are those implied by the wave-particle complementarity or duality principle. We have mentioned these complementarity relations in section 3.3, and we will examine them again in sections 6 and 7. This principle states that microparticles exhibit the properties of both particle and waves, even considering that, in classical physics, these categories are mutually exclusive. At the dawn of the XX century, physics had an assortment of phenomena that could not be appropriately explained by classical physics. In order to explain one of these phenomena, known as the photoelectric effect, Albert Einstein postulated in 1905, annus mirabilis, a model in which light, conceived in classical physics as electro-magnetic waves, should also be seen as a rain of tiny particles, now called photons. Einstein basic hypothesis was that a photon's energy is proportional to the light's frequency, $E = h\nu$, where the proportionality constant, h, is Planck's constant.

In 1924, Louis de Broglie generalized Einstein's hypotheses. Using Einstein's relativistic relation, $E = mc^2$, the photon's wavelength, $\lambda = c/\nu$, can be written as $\lambda = h/(mc)$, where $m = E/c^2$ is the effective mass attributed to the photon. A moving particle's moment is defined as the product of its mass and velocity, $p = mv$. Hence, de Broglie conjectured that any moving particle has associated to itself a "pilot wave" of wavelength $\lambda = h/p = h/(mv)$, see Broglie (1946, ch.IV, Wave Mechanics) for the original argument. Just two years later, in 1926, Erwin Schördinger published the paper "Quantization as an Eigenvalue Problem", further generalizing these ideas into his (Schördinger's) wave equation, the basis for a general theory of Quantum Mechanics, see next section. The details of the early developments of Quantum Mechanics can be found in Tomonaga (1962) and Pais (1988, ch.12), but from this brief history it is clear that the general idea of complementarity was a cornerstone in the birth of modern physics.

Nevertheless Bohr believed that complementarity could be a useful concept in many other areas. Folse (1985) gives an interesting essay about Bohr's ideas on complementarity, including its application to fields outside quantum mechanics. Possible examples of such applications are given next:

> *"...the lesson with respect to the role which the tools of observation play in defining the elementary physical concepts gives a clue to the logical applications of notions like purposiveness foreign to physics, but lending themselves so readily to the description of organic phenomena. Indeed, on this background it is evident that the attitudes termed mechanistic and finalistic do not present contradictory views on biological problems, but rather stress the mutually exhaustive observational conditions equally indispensable in our search for an ever richer description of life."* (Bohr II, Physical Science and Problems of Life, p.100).

"For describing our mental activity, we require, on one hand, an objectively given content to be placed in opposition to a perceiving subject, while, on the other hand, as is already implied in such an assertion, no sharp separation between object and subject can be maintained, since the perceiving subject also belongs to our mental content. From these circumstances follows not only the relative meaning of every concept, or rather of every word, the meaning depending upon our arbitrary choice of view point, but also we must, in general, be prepared to accept the fact that a complete elucidation of one and the same object may require diverse points of view which defy a unique description. Indeed, strictly speaking, the conscious analysis of any concept stands in a relation of exclusion to its immediate application. The necessity of taking recourse to a complementarity, or reciprocal, mode of description is perhaps most familiar to us from psychological problems. In opposition to this, the feature which characterizes the so-called exact sciences is, in general, the attempt to attain to uniqueness by avoiding all reference to the perceiving subject. This endeavor is found most consciously, perhaps, in the mathematical symbolism which sets up for our contemplation an ideal of objectivity to the attainment of which scarcely any limits are set, so long as we remain within a self-contained field of applied logic. In the natural sciences proper, however, there can be no question of a strictly self-contained field of application of the logical principles, since we must continually count on the appearance of new facts, the inclusion of which within the compass of our earlier experience may require a revision of our fundamental concepts. (Bohr I, The Quantum of Action, p.96-97).

Examining some basic concepts of quantum mechanics, L.V.Tarasov (1980, p.153) poses a question concerning the concept of complementarity that is very pertinent in our context:

"A microparticle is neither a corpuscle, nor a wave, but still we employ both these images, which mutually exclude each other, for describing a microparticle. ... Naturally, this could give rise to a ticklish question: Doesn't this mean an alienation of the image from the object, which is fraught with a transition to the position of subjectivism? A negative answer to this question is given by the principle of complementarity itself. From the position of this principle, pictures mutually excluding one another are used as mutually complementary pictures, adequately representing various sides of the objective reality called the microparticle."

Even considering that Tarasov makes his point from a very different epistemological perspective, his statement fits admirably well into our constructivist framework. Within it the objectivity of a complementarity model can be interpreted as follows: Although complementary, the several views employed to describe an object should still render objective

(epistemic) eigensolutions. As always, the whole model will be considered as objective as these well characterized eigensolutions, that is, sharp, stable, separable and composable, as examined in detail in section 3.5. Of course, the compositionality rules for a given theory or model must be given by an appropriate formalism. Such a formalism must include a full specification of compatibility / incompatibility rules for axioms or statements in the theory or model. For an example of this kind of formalism, see Costa and Krause (2004).

5.6 Varieties of Probability

This section presents some basic ideas of Quantum Mechanics, providing simple heuristic derivations for a few of its basic principles. Its main objective is to discuss the impact of Quantum Mechanics on the concept and interpretation of probability models.

5.6.1 Heisenberg's Uncertainty Principle

In this section we present Werner Heisenberg's uncertainty principle, derived directly from de Broglie's wave-particle complementarity principle.

A particle with a precise moment, p, has associated to it a pilot wave that is monochromatic, that is, has a single wavelength, λ. Hence, this wave is homogeneously distributed in space. Let us think of a particle with an uncertain moment, specified by a probability distribution, $\phi(p)$. What would the distribution, $\psi(x)$, of the location of its associated pilot wave, be? Assuming that the composition rule for pilot waves is the standard linear superposition principle, see Section 4.2, the answer to this question is given by the mathematics of Fourier series and transforms, see Butkov (1968, ch.4 and 7), Byron and Fuller (1969, ch.4 and 5) or Sadun (2001, ch.8 and 10).

The Fourier synthesis of a function, $f(x)$, in the interval $[0, L]$ is given by the Fourier series

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left(a_n \cos\left(\frac{n2\pi x}{L}\right) + b_n \sin\left(\frac{n2\pi x}{L}\right) \right) \ ,$$

$$a_n = \frac{2}{L} \int_0^L f(x) \cos\left(\frac{n2\pi x}{L}\right) dx \ , \quad b_n = \frac{2}{L} \int_0^L f(x) \sin\left(\frac{n2\pi x}{L}\right) dx \ .$$

The following examples give the Fourier series for the rectangular and triangular spike functions, $R_{2h}(x)$ and $T_{2h}(x)$. In order to obtain simpler expressions, the spikes are presented at the center of interval $[-\pi, +\pi]$, the standard interval of length $L = 2\pi$ shifted to be centered at the origin. Figure 10a displays the first 5 even harmonics, $\cos(nx)$, for wave number $n = 1 \ldots 5$, Figure 10b displays the Fourier coefficients, a_n, in the synthesis of the triangular spike $T_{2h}(x)$, for $h = 1.0$. Figures 10c and 10d display the triangular spike and its Fourier syntheses with the first 2 and the first 5 harmonics.
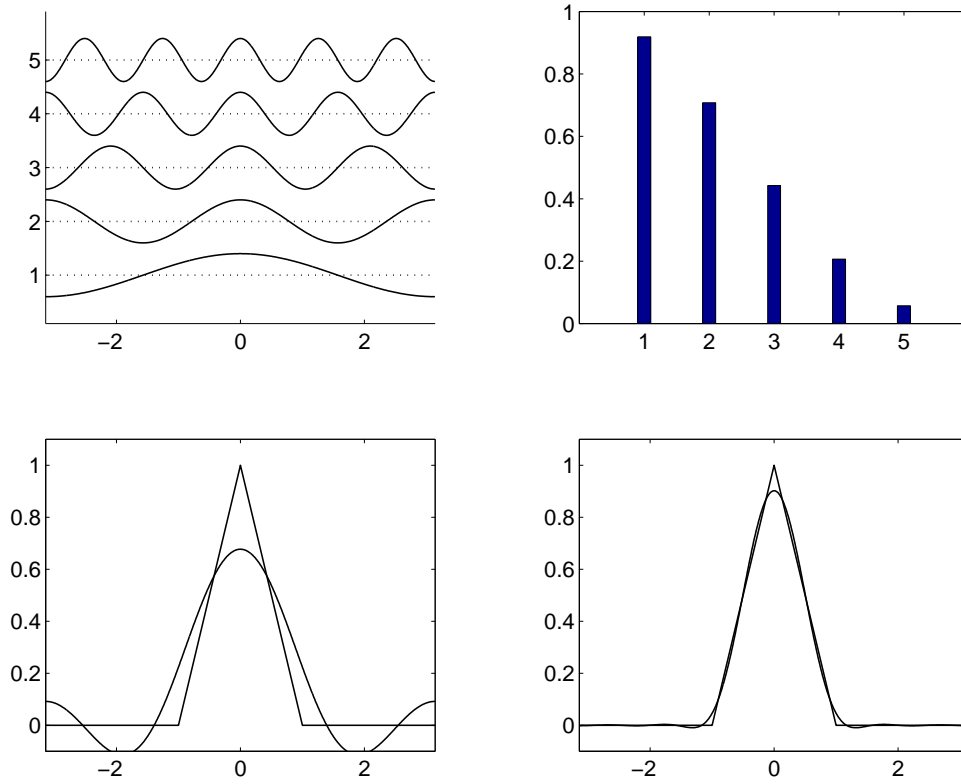
Figure 10: Monochromatic Waves and Superposition Packets.

$$R_{2h}(x) = \begin{cases} 1 \ , & \text{if } -h < x < +h, \\ 0 \ , & \text{otherwise in } [-\pi, \pi]. \end{cases} \quad = \quad \frac{2h}{\pi} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{\sin(nh)}{n} \cos(nx).$$

$$T_{2h}(x) = \begin{cases} 1 - |x|/h \ , & \text{if } |x| < h, \\ 0 \ , & \text{otherwise in } [-\pi, \pi]. \end{cases} \quad = \quad \frac{h}{2\pi} + \frac{4h}{\pi} \sum_{n=1}^{\infty} \left(\frac{\sin(nh)}{nh} \right)^2 \cos(nx).$$

It is also possible to express the Fourier series in complex form. Using the complex exponential notation, $\exp(ix) = \cos(x) + i\sin(x)$, we write

$$f(x) = \sum_{-\infty}^{+\infty} c_n e^{in2\pi x/L} \ , \quad c_n = \frac{1}{L} \int_0^L f(x) e^{-in2\pi x/L} dx \ \ .$$

The trigonometric and complex exponential Fourier coefficients are related as follows

$$c_0 = \frac{1}{2}a_0 \ \ , \quad c_n = \frac{1}{2}(a_n - ib_n) \ \ , \quad c_{-n} = \frac{1}{2}(a_n + ib_n) \ \ , \quad n = 1, \ldots \infty \ \ .$$

The complex form is more symmetric and elegant. In particular, the orthogonality relations,

$$\int_0^L e^{in2\pi x/L} e^{-im2\pi x/L} dx = \int_0^L e^{i(n-m)2\pi x/L} dx = \begin{cases} L , & \text{if } n = m , \\ 0 , & \text{if } n \neq m . \end{cases} ,$$

are the key for interpreting the set of complex exponentials, $\{e^{in2\pi x/L}\}$, for wave numbers $n = -\infty \ldots + \infty$, as an orthogonal basis for the appropriate functional vector space in the interval $[0, L]$.

If we want to synthetize functions in the entire real line, not just in a finite interval, we must replace Fourier series by Fourier transforms. The Fourier transform, $\widehat{f}(k)$, of a function, $f(x)$, and its inverse transform are defined, respectively, by

$$\widehat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \exp(-ikx) dx \quad \text{and} \quad f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widehat{f}(k) \exp(ikx) dk .$$

In the Fourier transform the propagation number (or angular frequency), $k = n2\pi/L$, replaces the wave number, n, used in the Fourier series. The new normalization constants are defined to stress the duality between the complementary representations of the function in state and frequency spaces, x and k.

As an important example, let us compute the Fourier transform, of a Gaussian distribution with mean $\mu = 0$ and standard deviation (uncertainty) $\sigma_x = \sigma$:

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(\frac{-x^2}{2\sigma^2}\right) , \quad \widehat{f}(k) = \frac{\sigma}{\sqrt{2\pi}} \exp\left(\frac{-\sigma^2 k^2}{2}\right) .$$

This computation can be checked using the analytic formula of the Gaussian integral,

$$\int_{-\infty}^{\infty} \exp\left(-ax^2 + bx + c\right) dx = \sqrt{\frac{\pi}{a}} \exp\left(\frac{b^2 - 4ac}{4a}\right) .$$
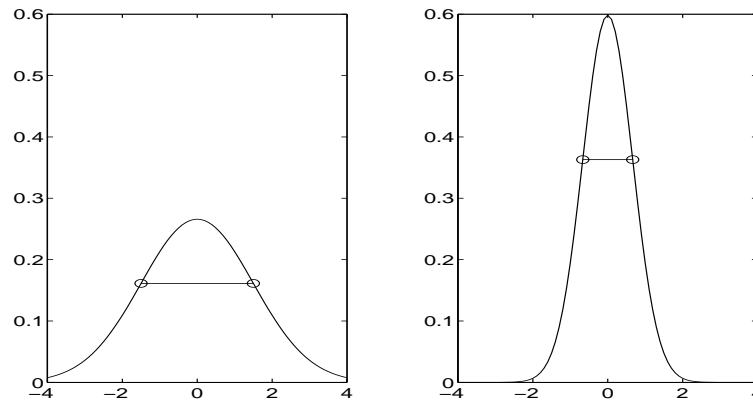
Figure 11: Uncertainty Relation for Fourier Conjugates.

Hence, the Fourier transform of a Gaussian distribution with standard deviation $\sigma_x = \sigma$, is again a Gaussian distribution, but with standard deviation $\sigma_k = 1/\sigma$, that is, $\sigma_x \, \sigma_k = 1$. Figure 11 displays the case $\sigma = 1.5$. It is also possible to show that this example is a best case, in the sense that, for any other function, $f(x)$, the standard deviations of the conjugate functions, $f(x)$ and $\widehat{f}(k)$, obey the inequality of the uncertainty principle, $\sigma_x \, \sigma_k \geq 1$, see Sadun (2001, sec.10.5).

In the context of Quantum Mechanics, the best known instance of the uncertainty principle gives a lower bound on the product of the standard deviations of the position and momentum of a particle,

$$\sigma_x \, \sigma_p \geq \frac{\hbar}{2} \;, \quad \hbar = \frac{h}{2\pi} \;, \quad h = 6.62606896(33)E-34 Js \;\;.$$

Heisenberg's bound is written as a function of the moment, p, instead of the frequency, k; this is why in the right hand side of the inequality we have half the reduced Planck's constant, $\hbar/2$, instead of 1, as in Fourier transform conjugate functions.

Planck's constant dimension is that of action, an energy-time product, like joule-second or electron-volt-second. The values above present the best current (2006) estimates for this fundamental physical constants, in the format recommended by the Committee on Data for Science and Technology, CODATA. The two digits in parentheses denote the standard deviation of the last two significant digits of the constant's value. The importance of this constant and its representation are further analyzed in the next sections.

5.6.2   Schrödinger's Wave Equation

In the last sections we have analyzed de Broglie's complementarity principle, which states that any moving particle has associated to itself a "pilot wave" of wavelength $\lambda = h/mv$. In section 4.2 we analyzed some of the basic properties of the classical wave equation, displayed below on the left hand side:

$$\frac{d^2\psi}{dx^2} + \omega^2 \, \psi = 0 \;\;, \quad \omega^2 = \frac{2m}{\hbar} \left(E - V(x) \right) \;\;.$$

In the classical equation, $\omega = 2\pi/\lambda$ is the wave's angular frequency. What should a quantum wave equation equation look like? Schrödinger's idea was to replace the classical wavelength by de Broglie's, that is, to use $\omega = 2\pi mv/h$. Using the definition of the kinetic energy of a particle, $T = (1/2)mv^2$, and its relation to $V(x)$ and E, the particle's potential and total energy, $T = E - V(x)$, we find the expression for ω^2 displayed above on the right.

This is Schrödinger's (time independent) wave equation, which established a firm basis for the development of Quantum Mechanics, also known in its early days as "wave mechanics". One of the immediate successes of Quantum Mechanics was to provide elegant

explanations, based of physical first principles, to many known empirical facts of chemistry, like the properties of the periodic table, molecular geometry, etc. Among the books providing accessible introductions to QM we mention: the very nice elementary text by Enge (1972), the concise introduction by Landshoff (1998), McGervey (1995) which focus on wave mechanics, and Heitler (1956) which focus on quantum chemistry.

Quantum Mechanics was also the basis for the development of completely new technologies. Among the most distinguished examples are solid-state or condensed matter electronic devices such as transistors, integrated circuits, lasers, liquid crystals, etc.. These devices constitute, in turn, the basic components of modern digital computers. Finally, one can argue that computer based information processing tools are among the most revolutionary technologies introduced in human society, having had an impact in its organization comparable only to a handful of other technologies (perhaps the steam and internal combustion engines, or electric power), see XX (20xx).

Nevertheless, all this success was not for free. Quantum Mechanics required the re-thinking and re-interpretation of some of the most fundamental concepts of science. In this and the next sections we analyze the impact of Quantum Mechanics on the most important concept of statistical science, namely, probability.

Although Scrödinger arrived at the appropriate functional form of a wave equation for Quantum Mechanics, the adequate interpretation for the wave function, ψ, was given only a few months later by Max Born. According to Born's interpretation: The probability density of "finding" the particle at position x, is proportional to the square of the wave function absolute amplitude, $|\psi(x)|^2$. Since, in the general case, ψ is a complex function, the last quantity can also be written as the product of the wave function by its complex conjugate, that is, $|\psi(x)|^2 = \psi^*\psi$.

From this interpretation of the wave function, we can understand Max Born's formulation of 'the core metaphor of wave mechanics', as quoted in Pais (1988, ch.12, sec.d, p.258),

> *"The essence of wave mechanics: 'The motion of particles follows probability laws but the probability itself propagates according to the law of causality."*

This is a revolutionary interpretation, that attributes to the concept of probability a new and distinct 'objective' character. Hence, it is interesting to have some insight on the genesis of Born's interpretation. Born's own recollections are presented at Pais (1988, ch.12, sec.d, p.258-259):

> *"What made Born take his step?*
> *In 1954 Born was awarded the Nobel Prize 'for his fundamental research, specially for his statistical interpretation of the wave function'. In his acceptance speech Born, then in his seventies, ascribed his inspiration for the*

statistical interpretation to 'an idea of Einstein's [who] had tried to make the duality of particles - light-quanta or photons - and waves comprehensible by interpreting the square of the optical wave amplitudes as probability density for the occurrence of photons. This concept could at once be carried over to the ψ-function: $|\psi|^2$ ought to represent the probability density of electrons.' "

5.6.3 Classic and Quantum Probability

One of the favorite metaphors used by the orthodox Bayesian school describes the scientist's work as a game against nature, with the objective of scoring a good guess on "nature's true state". Implicit in this metaphor is the assumption that such a "true state of nature" exists and is, at least in principle, accessible. In this paradigm, omniscience is usually a matter of money, that is, with enough economic resources all pertinent information can, at least in principle, be acquired, see Blackwell and Girshick (1954), for example.

> *"Statistics* can *be viewed as a game against nature." (p.75).*
> *"...games where one of the players is not faced with an intelligent opponent but rather with an unknown state of nature." (p.121).*
> *"The same theory that served to delineate optimal strategies in games played against an intelligent opponent will serve to delineate classes of optimal strategies in games played against nature." (p.123).*
> *"What prevents the statistician from getting full knowledge of ω [the state of nature] by unlimited experimentation is the cost of experiments." (p.78).*

This paradigm seems incompatible with, or at least very unfriendly to, Born's probabilistic interpretation of Quantum Mechanics and Heisenberg's uncertainty principle. We believe that, in the context of quantum mechanics, the strictly subjective interpretation of probability is, please forgive the pun, a very risky metaphor, and that pushing this metaphor where it does not belong will lead to endless paradoxes. In Chapter 7 of his book, *The Physics of Chance*, for example, Charles Ruhla presents the adventures of the simple-minded hero Monsieur de La Palice, struggling to understand some basic quantum experiments.

For a strict subjectivist the situation is even worse, and the use of Quantum Mechanics is at risk of being considered illegal. A statement giving the current best estimate of h (Planck's constant) together with its standard deviation was presented in section 5.6.1. Since h appears at the right hand side of Heisenberg's uncertainty principle, an uncertainty about the value of h implies a second order uncertainty. The propagation of the uncertainty about the value of fundamental physical constants generates similar second order probabilistic statements about the detection, mesurement or observation

of quantum phenomena. For example, section 5.7.2 arrives at statements giving the (probabilistic) uncertainty of (probabilistic) transition rates. All these are prototypical examples of statements that are categorically forbidden in orthodox Bayesian statistics, as bombastically proclaimed in the following quotations from Finetti (1977, p.1,5 and 1972, p.190), see also Mosleh and Bier (1996) and Wechsler et al. (2005).

> *"Does it make sense to ask what is the probability that the probability of a given event has a given value, p_i ? ... It makes* no *sense to state that the probability of an event E is to be regarded as* unknown *in that its* true *value is one of the p_i's, but we do not know which one."*
>
> *"Speaking of unknown probabilities [or of probability of a probability] must be forbidden as meaningless."*

A similar statement of de Finetti was analyzed in section 4.7. Such an awkward position, at least for a modern physicist, was seen by the founding fathers of orthodox Bayesian statistics as an unavoidable consequence of the subjectivist doctrine, according to which,

> *"Probabilities are states of mind, not of nature."* Savage (1981, p.674).

From a constructivist perspective, fundamental physical constants, including of course Planck's constant, correspond to very objective (very sharp, stable, separable and composable) eigenvalues of Physics' research program, and it is perfectly admissible to speak about the uncertainty of their estimated values. Of course that is what physicists need to do, and have done for almost a century, regardless of being disapproved by the Bayesian orthodoxy (theoretically coherent, but understandably very shy and timid). There have also been some attempts to reconcile a strict subjectivist position with modern physics, through long and sophisticated translations of simple "crude" statements like the ones quoted above. Some of these translations are as bizarre and / or intricately involved as similar attempts to translate epistemic probabilistic statements that are categorically forbidden in frequentist statistics into "acceptable" frequentist probabilistic statements, see section 2.5 and Rouanet et al. (1998, Preamble). Richard Feynman (2002, p.14), makes the following comments on some ideas behind some of such interpretations:

> *"Now, the philosophical question before us is, when we make an observation of our track in the past, does the result of our observation become real in the same sense that the final state would be defined if an outside observer were to make the observation? This is al very confusing, especially when we consider that even though we may consistently consider ourselves always to be the outside observer when we look at the rest of the world, the rest of the world is at the same time observing us, and that often we agree on what we*

see in each other. Does this mean that my observations become real only when I observe an observer observing something as it happens? This is an horrible viewpoint. Do you seriously entertain the thought that without observer there is no reality? Which observer? Any observer? Is a fly an observer? Is a star an observer? Was there no reality before 109 B.C. before life began? Or are you the observer? Then there is no reality to the world after you are dead? I know a number of otherwise respectable physicists who have bought life insurance. By what philosophy will the universe without man be understood?

In order to make some sense here, we must keep an open mind about the possibility that for sufficiently complex systems, amplitudes become probabilities...."

In order to provide deeper insight on the meaning of Heisenberg's uncertainty principle, let us link it to Noether's theorems, already discussed in section 2.8.1. The central point of Noether's theorems lies in the existence of an invariant physical quantity for each continuous symmetry group in a physical theory. Heisenberg's uncertainty relation, presented in section 6.1, sets a bound on the accuracy with which we can access, by means of physical measurements, such symmetry / invariant dual or conjugate pairs. This point is further analyzed by Bohr:

"...we admire Planck's happy intuition in coining the term 'quantum of action' which directly indicates a renunciation of the action principle, the central position of which in the classical description of nature he himself has emphasized on more than one occasion. This principle symbolizes, as it were, the peculiar reciprocal symmetry relation between the space-time description and the laws of conservation of energy and momentum, the great fruitfulness of which, already in classical physics, depends upon the fact that one may extensively apply them without following the course of the phenomena in space and time." (p.94 or 210).

"Indeed, the inevitability of using, for atomic phenomena, a mode of description which is fundamentally statistical arises from a closer investigation of the information which we are able to obtain by direct measurement of these phenomena and the meaning we may ascribe, in this connection, to the application of the fundamental physical concepts...

Such considerations lead immediately to the reciprocal uncertainty relations set up by Heisenberg and applied by him as the basis of a thorough investigation of the logical consistency of quantum mechanics." (p.113-114 or 247-248).

In the article *Space-Time Continuity and Atomic Physics*, Bohr (1935, p.370) further explores the relation between quantization and our use of probabilistic language:

> *"With the forgoing analysis we have described the new point of view brought forward by the quantum theory. Sometimes one has described it as leaving aside the idea of causality. I think we should rather say that in the quantum theory we try to express some laws of nature that lie so deep that they can not be visualized, or, which cannot be accounted for by the usual description in terms of motion. This state of affairs brings about the fact that we must use to a great extent statistical methods and speak of nature making choices between possibilities."*

The correct interpretation of probability has been one of the key conceptual problems of modern physics. The importance of this problem can be further appreciated in the following statement of Paul Dirac, found in (Pais 1986, p.255), regarding the early development of quantum mechanics:

> *"This problem of getting the interpretation proved to be rather more difficult than just working out the equations."*

The "correct" interpretation or "best" metaphysics for quantum mechanics, including the ontological and epistemological status of probability and the understanding of its role in the theory, is an area of strong academic interest and current research, see for example Albert (1993, ch.7) for an exposition of David Bohm's interpretation of QM. Richard Feynman's path integral formalism, see for example Feynman and Hibbs (1965), Honerkamp (1993) and Wiegel (1986), makes it possible to support other alternative interpretations.

Perhaps the most important lesson to be learned from this section is that one must be aware of the several possible meanings and interpretations of the concept of probability, and that distinct situations may require or benefit from distinct approaches. In the best spirit of complementarity, we should even consider the possibility of studying the same situation under different perspectives, each one of them providing a positive and irreplaceable contribution to our understanding of a whole that is beyond the grasp of a single picture [1].

5.7 Theories of Evolution

The objective of this section is to highlight the importance of three key concepts that are essential to modern theories explaining the evolution of complex systems, and to follow

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[1]The following quote was brought to my attention by Jean-Yves Beziau: "The ordinary man has always been sane because the ordinary man has always been a mystic... He has always cared for truth more than for consistency. If he saw two truths that seemed to contradict each other, he would take the two truths and the contradiction along with them." Gilbert Keith Chesterton (1874 - 1936).

some points in their development and interconnection, namely: (1) the systemic view; (2) modularity; and (3) stochastic evolution and/or probabilistic causation. Probabilistic causation is by far the most troublesome of these concepts. It is absolutely essential, at least in the framework presented in this chapter, to the evolution of complex systems, on one hand, but it was not easy for stochastic evolution to make its way as a "legitimate" concept in modern science, on the other. We believe that the historical progress and acceptance of the ontological status of these probabilistic concepts is closely related to the evolution of epistemological frameworks that can, in turn, strongly influence and be influenced by the corresponding statistical theories giving them operational support.

5.7.1　Systemic View and Probabilistic Causation

The systemic view has always been part of the biological thinking. The teleomechanics school gave particular importance to a systemic view of living organisms, see Lenoir (1989) for an excellent historical account. As quoted in Lenoir (1989, p.220,221), for example, the XVIII century biologist C. Reichert states:

> "…'we have a systemic product before us,… in which the intimate interconnections of the constituent parts have reached their highest degree. When we think about a system, we normally picture ourselves precisely this form of systematic product. Concerning such systems Kant said that the parts only exist with reference to the whole and the whole, on the other hand, only appears to exist for the sake of the parts.'
>
> In order to investigate the systematic character of biological organisms Reichert reminded the readers that it was necessary to have a method appropriate to the subject… Reichert could envision only one method to the investigation of the living organism which avoids disrupting the intimate interconnections of its parts:
>
> 'The systematist is aware both that he proceeds genetically and that he must proceed genetically. He is aware that the structure on an organism consists in the systematic division or dissection of the germ, which receives a particular systematic unity through inheritance, makes it explicit through development and transmits it further through procreation.' "

These statements express one of the core methodological doctrines of the teleomechanics school, namely, that to understand the systemic character of the organism, one must examine its development. The systemic approach of the teleomechanics school greatly contributed to the study of many fields in "Biology" (a word coined within this school), facilitating complex analyses and multiscale interconnections. C.F.Kielmeyer, another great representative of the teleomechanics school, for example, linked individual and pop-

ulational developments in his celebrated biogenic, parallelism, or recapitulation principle of Embryology:

> *"Ontogeny recapitulates phylogeny."*

The teleomechanics research program, however, could never overcome (perceived) incompatibility conflicts among some of its basic principles, such as, for example, the conflict between the teleological organization of organic systems, on one hand, and the need to use only scientifically accepted forms of causal explanation, on the other. Consequently the scientists in this program found themselves struggling between deterministic reductionist mechanisms and vitalistic explanations, both unable to offer significant scientific knowledge or acceptable understanding for the phenomena in study.

According to the framework for evolution presented in this chapter, the diagnostic for this failure is quite obvious, namely, the lack of key conceptual probabilistic ingredients. This situation is analyzed in Lenoir (1989, p.239-241):

> *"Only in a universe operating according to probabilistic laws, a universe grounded in non-deterministic causal processes, is it possible to harmonize the evolution of sequences of more highly organized beings with the principles of mechanics.*
>
> *Two paths lay open for providing a consistent and rigorous solution to this dilemma. One alternative is that of twentieth century science. It is simply to abandon the classical notion of cause in favor of a non-deterministic conception of causality. In the late nineteenth century this was not an acceptable strategy. To be sure statistical methods were being introduced into physics with great success, but prior to the quantum revolution in mechanics no one was prepared to assert the probabilistic nature of physical causes....*
>
> *A second solution to this dilemma is that proposed by teleomechanists. According to this interpretation rigidly determined causality can be retained, but then limits must be placed on the analysis of the ultimate origins of biological organization, and certain ground states of purposive or zweckmässig organization must be introduced.*
>
> *In the final analysis the only resolution of their impasse was the construction of an entirely new set of conceptual foundations for both the biological and the physical sciences which could cut the Gordian knot of chance and necessity."*

The breakthrough of introducing stochastic dynamics in modern theories of evolution is perhaps the greatest merit of Charles Darwin. According to Peirce (1893, 183-184):

> *"(In)* The origin of Species *published toward the end of 1859... the idea that chance begets order, which is one of the cornerstones of modern physics...*

was at that time put into its clearest light."

The role of probability in Darwin's theories can be best appreciated in his own words:

> *"Throughout this chapter and elsewhere I have spoken of selection as the paramount power, yet its action absolutely depends on what we in our ignorance call spontaneous or accidental variability. Let an architect be compelled to build an edifice with uncut stones, fallen from a precipice. The shape of each fragment may be called accidental; yet the shape of each has been determined by the force of gravity, the nature of the rock, and the slope of the precipice, -events and circumstances, all of which depend on natural laws ; but there is no relation between these laws and the purpose for which each fragment is used by the builder. In the same manner the variations of each creature are determined by fixed and immutable laws; but these bear no relation to the living structure which is slowly built up through the power of selection, whether this be natural or artificial selection.*
>
> *If our architect succeeded in rearing a noble edifice, using the rough wedge-shaped fragments for the arches, the longer stones for the lintels, and so forth, we should admire his skill even in a higher degree than if he had used stones shaped for the purpose. So it is with selection, whether applied by man or by nature; for although variability is indispensably necessary, yet, when we look at some highly complex and excellently adapted organism, variability sinks to a quite subordinate position in importance in comparison with selection, in the same manner as the shape of each fragment used by our supposed architect is unimportant in comparison with his skill."* Darwin (1887, ch.XXI, p.236)

In the above passage, the importance given to the systemic view, that is, to the *living structure of the organism* is evident. At the same time, randomness is added as an essential provider of raw materials in the evolutionary process. However, there are some important points of divergence between the way randomness plays a role in Darwinian evolution, and in contemporary theories. We highlight three of them: (1) Darwin uses only pseudo-randomness; (2) Genetic and somatic components of variation are not clearly distinguished; (3) Darwinian variations are continuous. Let us examine these three points more carefully:

1- Darwin used pseudo-randomness, not essential uncertainty. S.J.Gould (p.684) assesses this point is as follows:

> *"The Victorian age, basking in triumph of an industrial and military might rooted in technology and mechanical engineering, granted little conceptual space to random events... Darwin got into enough trouble by invoking randomness for sources of raw material; he wasn't about to propose stochastic causes for change as well!"*

As far as biological evolution is concerned, pseudo-randomness, as introduced by Darwin, is perfectly acceptable. The real need for the notion of "true" or objective probability, as in Quantum Mechanics, was still a few decades in the future.

2- Darwin didn't have a clear distinction between somatic versus genetic, or external versus internal, causes of variations. Winther (2000, p.425), makes the following comments:

> *"Darwin's ideas on variation, hereditarity, and development differ significantly from twentieth-century views. First, Darwin held that environmental changes, acting on the reproductive organs or the body, were necessary to generate variation. Second, hereditarity was a developmental, not a transmitional process..."*

At the time of Darwin, the available technology could not, of course, reveal the biochemical mechanisms of heredity. Nevertheless, scientists like Hugo de Vries and Erwing Schrödinger have had powerful insight on this mechanisms, even before the necessary technology became available. de Vries (1900), for example, advanced the following hypotheses:

> *"1. Protoplasm is made up of numerous small units, which are bearers of the hereditarity characters. 2. These units are to be regarded as identical with molecules."*

In his book *What is Life*, Schrödinger (1945) advanced more detailed hypotheses about the genetic coding mechanisms, based on far reaching theoretical insights provided by quantum mechanics. This small book was a declared source of inspiration for both James Watson and Francis Crick, who, in 1953, discovered the double-helix molecular structure of DNA, opening the possibility of deciphering the genetic code and its expression mechanisms.

3- Continuous variations. From several passages of Darwin's works, it is clear that he saw actual variations as coming from a continuum of potential possibilities:

> *"[as] I have attempted to show in my work on variation... they [are] extremely slight and gradual."* Darwin (1959, p.86).
> *"On the slow and successive appearence of new species: ...organic beings accord best with the common view of the immutability of species, or with that of their slow and gradual modification, through variation and natural selection."* Darwin (1959, p.167).
> *"It is indeed manifest that multitudes of species are related in the closest manner to other species that still exist, or have lately existed; and it will hardly be maintained that such species have been developed in an abrupt or*

sudden manner. Nor should it be forgotten, when we look to the special parts
of allied species, instead of to distinct species, that numerous and wonderfully
fine graduations can be traced, connecting together widely different structures."
Darwin (1959, p.117).

The first modern reference for discrete or modular genetic variations can be found
in the work of Gregor Mendel (1865), see next paragraph. It was unfortunate that the
ideas of Mendel, working at a secluded monastery in Brünn (Brno), were not immediately
appreciated. For a contemporary view of evolution and modularity, see Margulis (1999)
and Margulis and Sagan (2003).

> *"The Forms of the Hybrids:*
>
> *With some characters... one of the two parental characters is so prepon-*
> *derant that it is difficult, or quite impossible, to detect the other in the hybrid.*
>
> *This is precisely the case with the Pea hybrids. In the case of each of the*
> *7 crosses the hybrid-character resembles that of one of the parental forms so*
> *closely that the other either escapes observation completely or cannot be de-*
> *tected with certainty. This circumstance is of great importance in the determi-*
> *nation and classification of the forms under which the offspring of the hybrids*
> *appear. Henceforth in this paper those characters which are transmitted entire,*
> *or almost unchanged in the hybridization, and therefore in themselves consti-*
> *tute the characters of the hybrid, are termed the dominant, and those which*
> *become latent in the process recessive. The expression "recessive" has been*
> *chosen because the characters thereby designated withdraw or entirely disap-*
> *pear in the hybrids, but nevertheless reappear unchanged in their progeny, as*
> *will be demonstrated later on."*

The third point of divergence, variations discreteness, is, of course, closely linked with
the second, the nature of genetic coding. However, its implications are much deeper, as
examined in the next section.

5.7.2   Modularity Requires Quantization

The ideas of Herbert Simon about modularity, examined in section 3.2, seem to receive
empirical support from anywhere we look in the biological world. Ksenzhek and Volkov
(1998, p.80), also quoted in Souza and Manzatto (2000), for example, gives the following
example from Botany:

> *"A plant is a complicated, multilevel, hierarchical system, which provides a*
> *very high degree of integration, beginning from the elementary process of catch-*
> *ing light quanta and ultimately resulting in the functioning of a macroscopic*

Level	Size (m)	Structure	Transfer mechanism	Integration
1	$2E-8$	Chlorophyll antenna	Resonant exitons	300
2	$5E-7$	Tylakoid membrane	Electrochemical	500
3	$5E-6$	Cloroplast	Diffusion	50
4	$5E-5$	Cell	Diffusion, cyclosis	50
5	$2E-4$	Areolae	Diffusion	1E3
6	$1E-1$	Leaf	Hydraulics	1E5
7	$1-10$	Tree	Hydraulics	1E4

Table 3. Plant Energetics Hierachical and Modular Structure.

plant as an entire organism. The hierarchical structure of plants may be examined in a variety of aspects. (The following) table shows seven hierarchical levels of mass and energy."

As an example of how to interpret this table, we give further details concerning its first line: in a thylakoid membrane, about 300 chlorophyll molecules act like an antenna in a reaction center or photosynthetic unit, capable of absorbing light quanta at a rate of about 1K cycles / second. This energy conversion cycle absorbs photons of about $1.8eV$ (430 Hz or 700nm), synthesizing compounds, carbohydrates and oxygen, at an energy level of about $1.2eV$ higher than its input compounds, carbon dioxide and water.

Ksenzhek and Volkov (1998, p.80), see next quotation, also makes an important remark concerning the need for a specific and non-reductionist interpretation of each line in the above table, or structural level in the organism. For related aspects in Biology, see Buss (2007). Niels Bohr (1987b, Light and Life, p.3-12; Biology and Atomic Physics, p.13-22) presents a similar argument based on the general concept of complementarity.

"It should be noted that any hierarchical level that is above another level cannot be considered as the simple sum of the elements belonging to that lower level. In all cases, each step from a given level of the hierarchical staircase to the next one is followed by the development of new features not inherent in the elements of the lower level."

Table 2 stops at somewhat arbitrary levels and could be extended further up or down. Higher levels in the table would enter the domains of Ecology. Lower levels would penetrate the domains of Chemistry, and then Physics. At this point, we make an astonishing observation: Classical Physics *cannot* accommodate stable atomic models. Classical Physics gives *no* support for discreteness or modularity of any kind. Hence, our modular view of the world would be, within classical Physics, a giant with feet of clay! Werner Heisenberg (1958, p.5,6) describes the situation as follows:

"In 1911 Rutherford's observations... resulted in his famous atomic model.

The atom is pictured as consisting of a nucleus, which is positively charged and contains nearly the total mass of the atom, and electrons, which circle around the nucleus like planets circle around the sun. The chemical bond between atoms of different elements is explained as an interaction between the outer electrons of the neighboring atoms; it has not directly to do with the atomic nucleus. The nucleus determines the chemical behavior of the atom through its charge which in turn fixes the number of electrons in the neutral atom. Initially this model of the atom could not explain the most characteristic feature of the atom, its enormous stability. No planetary system following the laws of Newton's mechanics would ever go back to its original configuration after a collision with another such system. But an atom of the element carbon, for instance, will still remain a carbon atom after any collision or interaction in chemical binding.

The explanation of this unusual stability was given by Bohr in 1913, through the application of Planck's quantum hypothesis. An atom can change its energy only by discrete energy quanta, this must mean that the atom can exist only in discrete stationary states, the lowest of which is the normal state of the atom. Therefore, after any kind of interaction, the atom will finally always fall back into its normal state."
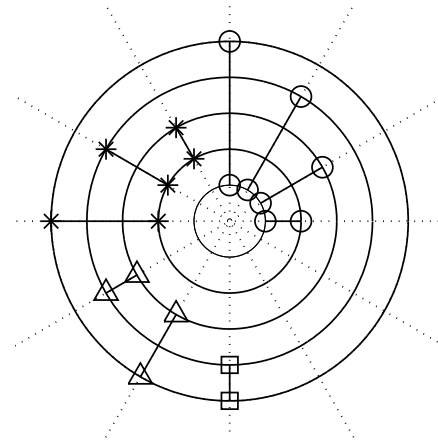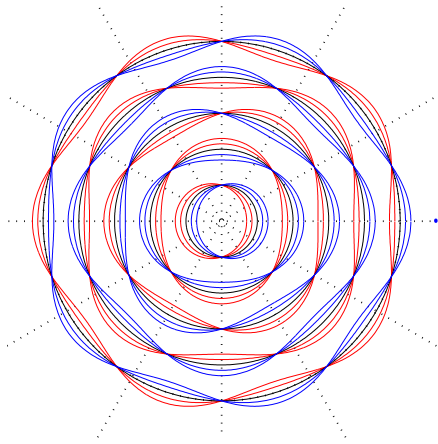
Figure 12: Orbital Eigensolutions for the Hydrogen Atom.
Figure 13: Orbital Transitions for Hydrogen Spectral Lines;
Series: Lyman, $n = 1$; Balmer, $n = 2$; Paschen, $n = 3$; $m = n + 1, \ldots \infty$.

Bohr's model is based on the quantization of the angular momentum of the electron in the planetary atomic model. The wave-particle duality metaphor can give us a simple visualization of Bohr's model. As already mentioned in section 4.2, a string of length L

with two fixed ends can only accommodate (stationary) waves whose (half) wavelength are a multiple of the string length, i.e. $L = n\lambda$, $n = 1, 2, 3, \ldots$. The first one ($n = 1$, longer wavelength, lower frequency) is called the fundamental frequency of the string, and the others ($n = 2, 3 \ldots$, shorter wavelengths, higher frequencies) are called its harmonics.

Putting together de Broglie's duality principle and the planetary atomic model, we can think of the electron's orbit as a circular string of length $L = 2\pi r$. Plugging in de Broglie's equation, $\lambda = h/mv$, and imposing the condition of having stable eigenfunctions or standing waves, see Enge (1972) and Figure 12, we have

$$2\pi r = n\lambda = \frac{nh}{m_e v} \quad \text{or} \quad m_e vr = n\frac{h}{2\pi} = n\hbar \ .$$

Planck's constant equals $6.626E - 34$ joule-seconds or $4.136E - 15$ electron-volt-second, and the electron mass is $9.11E - 28$ gram. Since the right hand side of this equation is the angular momentum of the orbiting electron, de Broglie wave-particle duality principle imposes its quantization.

Bohr's atomic model was also able to, for the first time, provide an explanation for another intriguing phenomenon, namely:

(a) Atoms only emit light at sharply defined frequencies, known as spectral lines;

(b) The frequencies, ν, or wavelengths, λ, of these spectral lines are related by integer algebraic expressions, like the Balmer-Rydberg-Ritz-Paschen empirical formula,

$$\frac{\nu_{n,m}}{c} = \frac{1}{\lambda_{n,m}} = R\left(\frac{1}{n^2} - \frac{1}{m^2}\right) \ ,$$

where $R = 1.0973731568525(73)E7 \ m^{-1}$ is Rydberg's constant.

Distinct combinations of integer numbers, $0 < n < m$, in BRRP formula give distinct wavelengths of the spectrum, see Enge (1972). It so happens that these frequencies are in precise correspondence with the differences of energy levels of orbital eigen-solutions, see Figure 13. These are the Hydrogen spectral series of Lyman, $n = 1$, Balmer, $n = 2$, Paschen, $n = 3$, and Brackett, $n = 4$, for $m = n + 1, \ldots \infty$. Similar spectral series have been known for other elements, and used by chemists and astronomers to identify the composition of matter from the light it radiates. Rydberg's constant can be written as $R = m_e e^4/(8\epsilon_0^2 h^3 c)$, where m_e is the rest mass of the electron, e is the elementary charge, ϵ_0 is the permittivity of free space, h is the Planck's constant, and c is the speed of light in vacuum.

The importance attributed by Bohr to the emergence of these sharp (discrete) eigen-solutions out of a higher dimensional continuum of possibilities is emphasized in Bohr (2007):

> *"Your physical aha-experience?*

> *Wavelengths of a complete series of spectral lines in the hydrogen spectrum can be expressed with the aid of integers. This information, he [Bohr] said, left an indelible impression on him."*

Approximation methods of perturbation theory can be used to compute probabilities of spontaneous and induced transitions between the different orbitals or energy states of an atom, and these transition rates can be observed as intensities of the respective spectral lines, see Enge (1972, ch.8), Landshoff (1998, ch.7) and McGervey (1995, ch.14). Comparative analyses between the value and accuracy of these theoretical calculations and empirical observations are of obvious interest. However, the natural interpretation of these analyses immediately generates statements about the uncertainty of transition rates, expressed as probabilities of probabilities. Hence, as explained in section 5.6.3, these statements collide with the canons of the subjectivist epistemological framework and are therefore unaceptable in orthodox Bayesian statistics.

5.7.3   Quantization Entails Objective Probability

An objective form of probability is at the core of quantum mechanics theory, as seen in previous sections. However, probabilistic explanations or probabilistic causation have been, at least from a historical perspective, very controversial concepts. This has been so since the earliest times. Aristotle (Physics, II,4,195b-196a) discusses events resulting from coincidences or incidental circumstances. If such an event serves a conscious human purpose, it is called $\tau \upsilon \chi \eta$, translated as luck or fortune. If it serves the "unconscious purposiveness of nature", it is called $\alpha \upsilon \tau o \mu \alpha \tau o \nu$, translated as chance or accident.

> *"We must inquire therefore in what manner luck and chance are present among the causes enumerated, and whether they are the same or different, and generally what luck and chance are.*
>
> *Thus, we must inquire what luck and chance are, whether they are the same or different, and how they fit into our division of causes.*
>
> *Some people even question whether they are real or not. They say that nothing happens by chance, but that everything which we ascribe to luck or chance has some definite cause.*
>
> *Others there are who, indeed, believe that chance is a cause, but that it is inscrutable to human intelligence, as being a divine thing and full of mystery."*

Aristotle (Physics, II,4,195b-196a) also reports some older philosophical traditions that made positive use of probabilistic causation, such as a stochastic development or evolution theory due to Empedocles:

> *"Wherever then all the parts came about just what they would have been if they had come be for an end, such things survived, being organized spon-*

> *taneously in a fitting way; whereas those which grew otherwise perished and continue to perish, as Empedocles says..."*

Many other ancient cultures accepted probabilistic arguments and/or did make use of randomized procedures, see Davis (1969), Kaptchuk and Kerr (2004) and Rabinovitch (1973). Even the biblical narrative, so averse to magic of any sort, presents the idea that destiny is ultimately inscrutable to human understanding, see for example Exodus (XXXIII, 18-23):

Moses, who is always willing to speak his mind, asks God for perfect knowledge:

> *And Moses said: I pray You, show me Your glory!*

In response God, Who is always ready to explain to Moses Who makes the rules, tells him that perfect knowledge can not be achieved by a living creature. This verse may also allegorically indicate that temporal irreversibility is a necessary consequence of such veil of uncertainty:

> *And the Lord said: You cannot see My face, for no man can see Me and live!...*
> *I will enclose and confine you, and protect you in My manner... (so that)*
> *You shall see My back, but My face shall not be seen.*

Nevertheless, the concepts of stochastic evolution and probabilistic causation lost prestige along the centuries. From the comments of Gould and Lenoir in section 7.1, we may conclude that at the XVIII and early XIX century its status reached the lowest level ever. It is ironic than that stochastic evolution is the concept at the eye of the storm of some of the most important scientific revolutions of the late XIX and XX century.

As seen in section 6, Quantum Mechanics entails Heisenberg's uncertainty principle, stating that we can not measure (in practice or in theory) the classical variables describing the motion of a particle with a precision beyond a hard threshold given by Planck's constant. Hence, the available information about a physical system is, in quantum mechanics, governed by *laws that are in nature essentially probabilistic*, or, as stated in Ruhla (1992, p.162),

> *"No longer is it chance as a matter of ignorance or of incompetence: it is chance quintessential and unavoidable."*

The path leading to an essentially stochastic world-view was first foreseen by people far ahead of their time, like C.S.Peirce and L.Bozmann, a path that was than advanced by reluctant revolutionaries like M. Planck, A. Einstein, and E. Schrödinger, who had a major participation in forging the new concept of probability, but that were at the same time, still emotionally attached to classical concepts. Finally, a third generation,

including N.Bohr, W.Heisenberg and M.Born fully embraced the new concept of objective probability. Of course, as with all truly innovative concepts, it will take mankind at least a few generations to truly assimilate and incorporate the new idea.

5.8   Final Remarks

The "objectification of probability" and the consequent raise of the ontological status of stochastic evolution and/or probabilistic causation was arguably one of the two greatest innovations of modern physics. The other great innovation is the "geometrization of space-time" in Einstein's theories of special and general relativity, see French (1968) and Martin (1988) for intuitive introductions, Sachs and Wu (1977) for a rigorous treatment, and Misner et al. (1973) for an encyclopedic treatise.

The manifestation of physical quantization and (special) relativistic geometry is regulated by Planck's constant and the speed of light. The value of these constants in standard (international) metric units, $h = 6.6E - 34\,Js$ and $c = 3.0E + 8\,m/s$, have, respectively, a tiny and huge order of magnitude, making it easy to understand why most of the effects of modern physics are not immediately perceptible in our ordinary life experience and, therefore, why classical physics can offer acceptable approximations in many circumstances of common statistical practice. However, modern physics has forever changed some of our most basic concepts related to space, time, causality and probability. Moreover, we have seen in this chapter how some of these concepts, like modularity and probabilistic causation, are essential to our theories and to understand phenomena in many other fields. We have also seen how quantization or stochastic evolution have a direct or indirect baring on areas much closer to our daily life, like Biology and Engineering. Hence, it is of vital importance to incorporate these new concepts to a contemporary epistemology or, at least, to use an epistemological framework that is not incompatible with these new ideas.

Chapter 6

The Living and Intelligent Universe

"Cybernetics is the science of defensible metaphors."

Gordon Pask (1928-1996).

"You, with all these words...."

Marisa Bassi Stern (my wife, when I speak too much).

"Yes I think to myself: What a wonderful world!"

B.Thiele and G.D.Weiss, in the voice of L.Armstrong.

In the article Mirror Neurons, Mirror Houses, and the Algebraic Structure of the Self, by Ben Goertzel, Onar Aam, F. Tony Smith and Kent Palmer (2008) and the companion article of Goertzel (2007), the authors provide an intuitive explanation for the logic of mirror houses, that is, they study symmetry conditions for specular systems entailing the generation of kaleidoscopic images. In these articles, the authors share (in my opinion) several important insights on autopoietic systems and constructivist philosophy. A more prosaic kind of mirror house used to be a popular attraction in funfairs and amusement parks. The entertainment then came from misperceptions about oneself or other objects. More precisely, from the misleading ways in which a subject sees how or where are the objects inside the mirrorhouse, or how or where himself stands in relation to other objects.

The main objective of this chapter is to show how similar misperceptions in science can lead to ill-posed problems, paradoxical situations and even misconceived philosophi-

cal dilemmas. The epistemological framework of this discussion will be that of cognitive constructivism, as presented in previous chapters. In this framework, objects within a scientific theory are tokens for eigen-solutions which Heinz von Foerster characterized by four essential attributes, namely those of being discrete (precise, sharp or exact), stable, separable and composable. The Full Bayesian Significance Test (FBST) is a possibilistic belief calculus based on a (posterior) probabilistic measure originally conceived as a statistical significance test to assess the objectivity of such eigen-solutions, that is, to measure how well a given object manifests or conforms to von Foerster's four essential attributes.

The FBST belief or credal value of hypothesis H given the observed data X is the *e-value*, $\text{ev}(H \,|\, X)$, interpreted as the *epistemic value* of hypothes H (given X), or the *evidence value* of data X (supporting H). A formal definition of the FBST and several of its implementations for specific problems can be found in the author's previous articles, and summarized in appendix A. From now on, we will refer to Cognitive Constructivism accompanied by Bayesian statistical theory and its tool boxes, as laid down in the aforementioned articles, as the Cog-Con epistemological framework.

Instead of reviewing the formal definitions of the essential attributes of eigen-solutions, we analyze instead the Origami example, a didactic case presented by Richard Dawkins. This is the done in section 1. The origami example is so simple that it may look trivial and, in some sense, it is so. In subsequent sections we analyze in which ways the eigen-solutions found in the practice of science can be characterized as non-trivial, and also highlight some (in my view) common misconceptions about the nature of these non-trivial objects, just like distinct forms of illusion in a mirror-house.

In section 2 we contrast the control, precision and stability of morphogenic folding processes in autopoietic and allopoietic systems. In section 3 we concentrate in object orientation and code reuse, inter-modular adaptation and resonance, and also analyze the yoyo diagnostic problem. In section 4 we explore auto-catalytic and hypercyclic networks, as well as some related bootstrapping paradoxes. This section is heavily influenced by the work of Manfred Eigen. Section 5 focus on explanations of specific components, single links or partial chains in long cyclic networks, including the meaning of some forms of directional (such as upward or downward) causation. In section 6 we study the emergence of asymptotic eigen-solutions such as thermodynamic variables or market prices, and in section 7 we analyze the ontological status of such entities. In section 8 we study the limitations in the role and scope of conceptual distinctions used in science, and the importance of probabilistic causation as a mechanism to overcome, in a constructive way, some of the resulting dilemmas. In short, section 2 to 8 discus autopoiesis, modularity, hypercycles, emergence, and probability as sources of complexity and forms of non-trivial organization. Our final remarks are presented in section 9.

In this chapter we have made a conscious effort to use examples that can be easily

visualized in space and time scales directly perceptible to our senses, or at least as close as possible to it. We have also presented our arguments using, whenever possible, very simple (high school level) mathematics. We did so in order to make the examples intuitive and easy to understand, so that we could concentrate our attention on the epistemological aspects and difficulties of the problems at hand. Several interesting figures and images that illustrate some of the concepts discussed in this chapter are contained in the website `www.ime.usp.br/~jstern/pub/gallery2.pdf/` .

6.1 The Origami Example

The Origami example, from the following text in Blackmore (1999, p.x-xii, emphasis are ours) was given by Richards Dawkins to present the notion of reliable replication mechanisms in the context of evolutionary systems. Dawkins' example contrasts two versions of the Chinese Whispers game using distinct copy mechanisms.

Suppose we assemble a line of children. A picture, say, a Chinese junk, is shown to the first child, who is asked to draw it. The drawing, but not the original picture, is then shown to the second child, who is asked to make her own drawing of it. The second child's drawing is shown to the third child, who draws it again, and so the series proceeds until the twentieth child, whose drawing is revealed to everyone and compared with the first. Without even doing the experiment, we know what the result will be. The twentieth drawing will be so unlike the first as to be unrecognizable. Presumably, if we lay the drawings out in order, we shall note some resemblance between each one and its immediate predecessor and successor, but the mutation rate will be so high as to destroy all semblance after a few generations. A trend will be visible as we walk from one end of the series of drawings to the other, and the direction of the trend will be degeneration...

High fidelity is not necessarily synonymous with digital. Suppose we set up our Chinese Whispers Chinese Junk game again, but this time with a crucial difference. Instead of asking the first child to copy a drawing of the junk, we teach her, by demonstration, to make an origami model of a junk. When she has mastered the skill, and made her own junk, the first child is asked to turn around to the second child and teach him how to make one. So the skill passes down the line to the twentieth child. What will be the result of this experiment? What will the twentieth child produce, and what shall we observe if we lay the twenty efforts out in order along the ground? ...

In several of the experiments, a child somewhere along the line will forget some crucial step in the skill taught him by the previous child, and the line of phenotypes will suffer an abrupt macromutation which will presumably then

be copied to the end of the line, or until another discrete mistake is made. The end result of such mutated lines will not bear any resemblance to a Chinese junk at all. But in a good number of experiments the skill will correctly pass all along the line, and the twentieth junk will be no worse and no better, on average, than the first junk. If we lay then lay the twenty junks out in order, some will be more perfect than others, but imperfections will not be copied on down the line...

Here are the first five instructions... for making a Chinese junk:

1. Take a *square* sheet of paper and fold all four corners *exactly* into the *middle*.

2. Take the reduced *square* so formed, and fold one side into the *middle*.

3. Fold the opposite side into the *middle, symmetrically*.

4. In the same way, take the *rectangle* so formed, and fold its two ends into the *middle*.

5. Take the small *square* so formed, and fold it backwards, *exactly* along the *straight line* where you last two folds met...

These instructions, though I would not wish to call them digital, are potentially of very high fidelity, just as if they were digital. This is because they all make reference to idealized tasks like 'fold the four corners exactly into the middle'... The instructions are self-normalizing. The code is error-correcting...

Dawkins recognizes that instructions for constructing an origami have remarkable properties, providing the long term survival of the subjacent *meme*, i.e. specific model or single idea, expressed as an origami. Nevertheless, Dawkins is not sure how he "wishes to call" these properties (digital? high fidelity?). What adjectives should we use to appropriately describe the desirable characteristics that Dawkins perceives in these instructions? I claim that von Foerster's four essential attributes of eigen-solutions offer an accurate description of the properties relevant to the process in study.

The instructions and the corresponding (instructed) operations are precise, stable, separable and composable. A simple interpretation of the meaning of these four attributes in the origami example is the following:

Precision: An instruction like "fold a paper joining two opposite corners of the square" implies that the folding must be done along a diagonal of the square. A diagonal is a specific line, a 1-dimensional object in the 2-dimensional sheet of paper. In this sense the instruction is precise or exact.

Stability: By interactively adjusting and correcting the position of the paper (before making a crease) it is easy to come very close to what the instruction specifies. Even if the resulting fold is not absolutely perfect (in practice it actually never is), it will probably still work as intended.

Composability and Separability: We can compose or superpose multiple creases in the same sheet of paper. Moreover, adding a new crease will not change or destroy the existing ones. Hence, we can fold them one at a time, that is, separately.

These four essential attributes are of fundamental importance in order to understand scientific activity in the Cog-Con framework. Moreover, Dawkins' origami example illustrates these attributes with striking clarity and simplicity.

In the following sections we will examine other examples, which are less simple, not so clear or non-trivial in a distinct and characteristic way. We will also draw attention to some confusions and mistakes often made when analyzing systems with similar characteristics.

6.2 Autopoietic Control, Precision, Stability

The origami folding is performed and controlled by an external agent, the person folding the paper. In contrast, organic development processes are self-organized. These processes are not driven by an external agent, do not require external supervision, and usualy are not even amenable to external corrections. While artifacts and machines manufactured like an origami are called *allopoietic*, from $\alpha\lambda\lambda o\text{-}\pi o\iota\eta\sigma\iota\varsigma$ - external production, living organisms are called *autopoietic*, from $\alpha\upsilon\tau o\text{-}\pi o\iota\eta\sigma\iota\varsigma$ - self production.

Autopoiesis is a non-trivial process, in many interesting ways. For example, the inexistence of external supervision or correction mechanism requires an autopoietic process to be stable. Moreover, typical biological processes occur in environments with high levels of noise and have large (extra) variability. Hence the process must be intrinsically self-correcting and redundant so that its noisy implementation does not compromise the viability of the final product.

6.2.1 Organic Morphogenesis: (Un)Folding Symmetries

In this section we make some considerations about morphogenic biological processes, namely, we study examples of tissue folding in early embryonic development. This process naturally invites not only strong analogies, but also sharp contrasts with the origami example. At a macroscopic (supra cellular) level, the organisms' organs and structures are built by tissue movements, as described in Forgacs and Newman (2005, p.109), and Saltzman (2004, p.38).

The main types of tissue movements in morphogenic process are:

- Epiboly: spreading of a sheet of cells over deeper layers.

- Emboly: inward movement of cells which is of various types as:

- Invagination: infolding or insinking of a layer,

- Involution: inturning, inside rotation or inward movement of a tissue.

- Delamination: splitting of a tissue into 2 or more parallel layers.

- Convergent/Divergent Extension: stretching together/apart of two distinct tissues.

The blastula is an early stage in the embryonic development of most animals. It is produced by cleavage of a fertilized ovum and consists of a hollow sphere of around 128 cells surrounding a central cavity. From this point on, morphogenesis unfolds by successive tissue movements. The very first of such moves is known as gastrulation, a deep invagination producing a tube, the archenteron or primitive digestive tract. This tube may extend all the way to the pole opposing the invagination point producing a second opening. The opening(s) of the archenteron become mouth and anus of the developing embryo.

Gastrulation produces three distinct (germ) layers, that will further differentiate into several body tissues. Ectoderm, the exterior layer, will further differentiate into skin and nervous systems. Endoderm, the innermost layer at the archenteron, generates the digestive system. Mesoderm, between the ectoderm and endoderm, differentiates into muscles, connective tissues, skeleton, kidneys, circulatory and reproductive organs. We will use this example to highlight some important topics, some of which will be explored more thoroughly in further sections.

Discrete vs. Exact or Precise Symmetries

Notice that origami instructions, that implicitly rely on the *symmetries* characterizing the shape of the paper, require foldings at sharp edges or cresses. Hence, a profile of the folded paper sheet may look like it breaks (is non-differentiable) at a discrete or singular point.

Organic tissue foldings have no sharp edges. Nevertheless, the (idealized) symmetries of the folded tissues, like the spherical symmetry of the blastula, or the cylindrical symmetry of the gastrula, can be described by equations just as exact or precise, see Beloussov (2008), Nagpal (2002), Odel et al. (1980), Tarasov (1986), and Weliky and Oster (1990). This is why we usually prefer the adjectives *precise* or *exact* to the adjective *discrete* used by von Foester in his original definition of the four essential properties of an eigen-solution.

Centralized vs. Decentralized Control

In morphogenesis, there is no agent acting like a central controller, dispatching messages ordering every cell what to do. Quite the opposite, the complex forms and tissue move-

ments at a global or macroscopic (supra cellular) scale are the result of collective cellular behavior patterns based on distributed control. The control mechanisms rely on simple local interaction between neighboring cells, see Keller et al. (2003), Koehl (1990), and Newman and Comper (1990). Some aspects of this process are further analyzed in sections 3 and 6.

6.3   Object Orientation and Code Reuse

At the microscopic level, cells at the several organic tissues studied in the last section are differentiated by distinct metabolic reaction patterns. However, the genetic code of any individual cell in a organism is identical (as always in biology, there are exceptions, but they are not relevant to this analysis), and cellular differentiation at distinct tissues are the result of differentiated (genetic) expressions of this sophisticated program.

As studied in Chapter 5, complex systems usually have a modular hierarchical structure or, in computer science jargon, an object oriented design. In allopoietic systems object orientation is achieved by explicit design, that is, it has to be introduced by a knowledgeable and disciplined programmer, see Budd (1999). In autopoietic systems modularity is an implicit and emergent property, as analyzed in Angeline (1996), Banzaff (1998), Iba (1992), Lauretto at al. (2009) and Chapter 5.

Object oriented design entails the reuse, over and over, of the same modules (genes, functions or sub-routines) as control mechanisms for different processes. The ability to easily implement this kind of feature was actively pursued in computer science and software engineering. Object orientation was also discovered, with some surprise, to be naturally occurring in developmental biology, see Carrol (2005).

However, like any abused feature, code reuse can also become a burden in some circumstances. The difficulty of locating the source of a functionality (or a bug) in an intricate inheritance hierarchy, represented by a complex dependency graph, is known in computer science as the yoyo problem. According to the glossary in Budd (1999, p.408), "Yoyo problem: Repeated movements up and down the class hierarchy that may be required when the execution of a particular method invocation is traced."

Systems undergoing many changes or modifications, under repeated adaptation or expansion, or on rapid evolution are specially vulnerable to yoyo effects. Unfortunately, the design of the human brain and its mental abilities are under all of the above conditions. In the next subsection we study some examples in this area, related to biological neural networks and language. These examples also include some mental dissociative phenomena that can be considered as manifestations of the yoyo problem.

6.3.1   Doing, Listening and Answering

In this section we study some human capabilities related to doing (acting), listening (linguistic understanding) and answering (dialogue). The capabilities we have chosen to study are related to the phylogenetic acquisition and the ontogenetic development of:
- Mechanisms for precision manipulation, production of speech and empathic feeling;
- Syntax for complex manipulation procedures, language articulation and behavioral simulation;
- Semantics for action, communication and dialogue; and the learning of
- Technological know-how, social awareness and self-awareness.

When considering an action in a modern democratic society, we usually deliberate what to do (unless there is already a tacit agreement). We then communicate with other agents involved to coordinate this action, so that we are finally able to do what has to be done. Evolution, it seems, took exactly the other way around. Phylogenetically, the path taken by our species follows a stepwise development of several mechanisms (that were neither independent nor strictly sequential), including:

1. A mechanism for 3-dimensional vision and precision measurement, fine motor control of hands and mouth, and visual-motor coordination for the complex procedures of *precision manipulation*.

2. Mechanisms for *imitating*, *learning* and *simulating* the former procedures or actions.

3. Mechanisms for *simulating* (possible) actions taken by other individuals, their consequences and motivations, that is, mechanisms for awareness and (behavioral) understanding of other individuals.

4. A mechanism for *communicating* (possible) actions, used for commanding, controlling and coordinating group actions. The use of such a mechanism implies a degree of awareness of others, that is, some ability to communicate, explain, listen and learn what you do, *you* - an agent like *me*.

5. Mechanisms for *dialoging* and *deliberating*, that is, for negotiating, goal selecting and non-trivial social planning. The use of such mechanisms implies some *self-awareness* or *consciousness*, that is, the conceptualization of an ego, an abstract *I* - an agent like *you*.

In a living individual, all of these mechanisms must be well integrated. Consequently, it is natural that they work using coherent implicit grammars, reflecting compatible subjacent rules of composition for action, language and inter-individual interaction. Indeed, resent research in neuro-science confirm the coherence of these mechanisms. Moreover, this research shows that this coherence is based not just on compatible designs of separate systems, but on intricate schemes of use and reuse of the same structures, namely, the firmware code or circuits implemented as biological neural networks.

Mirror neuron is a concept of neuroscience that highlights the reuse of the same circuits for distinct functions. A mirror neuron is part of a circuit which is activated (fires) when an individual executes an action, and also when the individual observes another individual executing the same action as if he, the observer, were performing the action himself. The following passages, from important contemporary neuro-scientists, give some hints on how the mechanisms mentioned in the past paragraph are structured.

The first group of quotes, from Hesslow (2002, p.245), states the mirror neuron *simulation hypothesis*, according to which, the same circuits used to control our actions are used to learn, simulate, and finally "understand" possible actions taken by other individuals. According to the simulation hypothesis, we are then naturally endowed with the capability of observing, listening, and "reading the mind" of (that is - understanding, by simulation, the meaning or intent of the possible actions taken by) our fellow human beings.

> ...the simulation hypothesis states that thinking consists of simulated interaction with the environment and rests on the following three core assumptions:
> (1) simulation of actions: we can activate motor structures of the brain in a way that resembles activity during a normal action but does not cause any overt movement;
> (2) simulation of perception: imagining perceiving something is essentially the same as actually perceiving it, only the perceptual activity is generated by the brain itself rather than by external stimuli;
> (3) anticipation: there exist associative mechanisms that enable both behavioral and perceptual activity to elicit other perceptual activity in the sensory areas of the brain. Most importantly, a simulated action can elicit perceptual activity that resembles the activity that would have occurred if the action had actually been performed. (p.5).

> In order to understand the mental state of another when observing the other acting, the individual imagines herself/himself performing the same action, a covert simulation that does not lead to an overt behavior. (p.5).

The second group of quotes, from Rizzolatti and Arbib (1998), states the mirror neuron *linguistic hypothesis*, according to which, the same structures used for action simulation, are reused to support human language.

> Our proposal is that the development of the human lateral speech circuit is a consequence of the fact that the precursor of Broca's area was endowed, before speech appearance, with a mechanism for recognizing actions made by others. This mechanism was the neural prerequisite for the development of inter-individual communication and finally of speech. We thus view language

in a more general setting than one that sees speech as its complete basis. (Rizzo.p.190).

...a 'pre-linguistic grammar' can be assigned to the control and observation of actions. If this is so, the notion that evolution could yield a language system 'atop' of the action system becomes much more plausible. (p.191).

In conclusion, the discovery of the mirror system suggests a strong link between speech and action representation. 'One sees a distinctly linguistic way of doing things down among the nuts and bolts of action and perception, for it is there, not in the remote recesses of cognitive machinery, that the specifically linguistic constituents make their first appearance'. (p.193-194).

Finally, a third group of quotes, from Ramachandran (2007), states the mirror neuron *self-awareness hypothesis*, according to which, the same structures used for action simulation are reused, over again, to support abstract concepts related to consciousness and self-awareness. According to this perspective, perhaps the most important of such concepts, that of an abstract self-identity or ego, is built upon one's already developed simulation capability for looking at oneself as if looking at another individual.

I suggest that 'other awareness' may have evolved first and then counter-intuitively, as often happens in evolution, the same ability was exploited to model one's own mind - what one calls self awareness.

How does all this lead to self awareness? I suggest that self awareness is simply using mirror neurons for 'looking at myself as if someone else is look at me' (the word 'me' encompassing some of my brain processes, as well).

The mirror neuron mechanism - the same algorithm - that originally evolved to help you adopt another's point of view was turned inward to look at your own self. This, in essence, is the basis of things like 'introspection'.

This in turn may have paved the way for more conceptual types of abstraction; such as metaphor ('get a grip on yourself').

Yoyo Effects and the Human Mind

From our analyses in the preceding sections, one should expect, as a consequence of the heavy reuse of code under fast development and steady evolution, the sporadic occurrence of some mental yoyo problems. Such yoyo effects break the harmonious way in which the same code is (or circuits are) supposed to work as an integral part with several functions used to *do*, *listen* and *answer*, that is, to control action performance, language communication, and self or other kind of awareness. In psychology, many of such effects are known

as *dissociative phenomena.* For carefully controlled studies of low level dissociative phenomena related to corporal action-perception, see Schooler (2002) and Johansson et al. (2008).

In the following paragraphs we give a glimpse on possible neuroscience perspectives of some high level dissociative phenomena. Simulation mechanisms are (re)used to simulate one's actions, as well as other agents' actions. Contextualized action simulation is the basis for intentional and motivational inference. From there, one can assess even higher abstraction levels such as tactical and strategic thinking, or even ethics and morality. But these capabilities must rely on some principle of decomposition, that is, the ability to separate, to some meaningful degree, one's own mental state from the mental state of those whose behavior is being simulated. This premise is clearly stated in Decety and Grèzes (2005, p.5):

> One critical aspect of the simulation theory of mind is the idea that in trying to impute mental states to others, an attributor has to set aside her own current mental states and substitute those of the target.

Unfortunately, as seen in the preceding section, the same low level circuits used to support simulation are also used to support language. This can lead to conflicting requests to use the same resources. For example, verbalization requires introspection, a process that conflicts with the need to set aside one's own current mental state. This conflict leads to *verbal overshadowing* - the phenomenon by which verbally describing or explaining an experienced or simulated situation somehow modifies or impairs its correct identification (like recognition or recollection), or distorts its understanding (like contextualization or meaning). Some causes and consequences of this kind of conflict are addressed by Iacoboni (2008, p.270):

> Mirror neurons are pre-motor neurons, remember, and thus are cells not really concerned with our reflective behavior. Indeed, mirroring behaviors such as the chameleon effect seem implicit, automatic, and pre-reflexive. Meanwhile, society is obviously built on explicit, deliberate, reflexive discourse. Implicit and explicit mental processes rarely interact; indeed, they can even dissociate. (p.270).

Psychoanalysis can teach us a lot about high level dissociations such as emotional / rational psychological mismatches and individual / social behavioral misjudgments. For a constructivist perspective of psychotherapy see Efran et al. (1990), and further comments on section 7.

We end up this section by posing a tricky question capable of inducing the most spectacular yoyo bouncings. This provocative question is related to the role played by division

algebras; Goertzel's articles mentioned at the introduction provide a good source of references. Division algebras capture the structure of eigen-solutions entailed by symmetry conditions for the recursively generated systems of specular images in a mirror house. The same division algebras are of fundamental importance in many physical theories, see Dion et al. (1995), Dixon (1994) and Lounesto (2001). Finally, division algebras capture the structure of 2-dimensional (complex numbers) and 3-dimensional (quaternion numbers) rotations and translations governing human manipulation of objects, see Hanson (2006). We can thus ask: Do we keep finding division algebras everywhere out there when trying to understand the physical universe because we already have the appropriate hardware to see them, or is it the other way around? We can only suspect that any trivial choice in the dilemma posed by this trick question, will only result in an inappropriate answer. We shall revisit this theme at sections 7 and 8.

6.3.2   Mnemes, Memes, Mimes, and all that.

We can make the ladder of hierarchical complexity in the systems analyzed in the last sections go even further up, as if it did not climb high enough, by including new steps in the socio-cultural realms that stand above the level of simple or direct inter-individual interaction, such as art, law, religion, science, etc. The origami example of section 1 is used by Richard Dawkins as a prototypical *meme* or a unit of imitation. The term *mneme*, derived from $\mu\nu\eta\mu\eta$, the muse of memory, was used by Richard Semon as a unit of retrievable memory. Yet another variant of this term, *mime*, is derived from $\mu\iota\mu\eta\sigma\iota\varsigma$ or imitation. All these terms have been used to suggest a basic model, a single concept, an elementary idea, a memory trace or unit, or to convey related meanings, see Blackmore and Dawkins (1999), Dawkins (1976), van Driem (2007), Schacter (2001), Schacter et al. (1978), and Semon (1904, 1909, 1921, 1923).

Richard Semon's theory was able to capture many important characteristics concerning the storage or memorization, retrieval, propagation, reproduction and survival of mnemes. Semon was also able to foresee many important details and interconnections, at a time when there were no experimental techniques suitable for an empirical investigation of the relevant neural processes. Unfortunately, Semon's analysis also suffers from the yoyo effect in some aspects. That is not surprising at all given the complexity of the systems he was studying and the lack of suitable experimental tools. These yoyo problems were related to some mechanisms, postulated by Semon, for mnemetic propagation across generations, or mnemetic hereditarity. Such mechanisms had a Lamackian character, since they implied the possibility of hereditary transmission of learned or acquired characteristics.

In modern Computer Science, the term *memetic algorithm* is used to describe evolutive programming based on populational evolution by code (genetic) propagation that combines a Darwinian or selection phase, and a local optimization or Lamackian learning phase, see Moscato (1989). Such algorithms were inspired by the evolution of ideas and

culture in human societies, and they proved to be very efficient for solving some complex combinatorial problems, see Ong et al (2007) and Smith (2007). Consequently, even knowing now, based on contemporary neural science, that some of the concepts developed by Semon are not appropriate to explain specific phenomena among those he was studying, he was definitely postulating, far ahead of his time, some very interesting and useful ideas.

Nevertheless, for Semon's misfortune, he published his theory at the aftermath of the great Darwinian victory over the competing Lamarckian view in the field of biological evolution. At that time, any perceived contamination by Lamackian ideas was a kiss of death for a new theory, even if postulated within a clearly distinct context. As a regrettable consequence, the mneme concept was rejected and cast into oblivion for half a century, until its revival as Dawkin's meme. Such a drama is by no means unusual in the history of science. It seems that some ideas, postulated ahead of their time, have to be incubated and remain dormant until the world is ready for them. Another example of this kind, related to the concept of statistical randomization, is analyzed in great detail in Chapter 3.

6.4 Hypercyclic Bootstrapping

On march 1st 2009, the Wikipedia definition for bootstrapping read:

> Bootstrapping or booting refers to a group of metaphors that share a common meaning, a *self-sustaining* process that proceeds without external help. The term is often attributed to Rudolf Erich Raspe's story The Adventures of Baron Münchausen, where the main character pulls himself out of a swamp, though it's disputed whether it was done by his hair or by his bootstraps.

The attributed origin of this metaphor, the (literally) incredible adventures of Baron Münchhausen, well known as a compulsive liar, makes us suspect that there may be something wrong with some of its uses. There are, however, many examples where bootstrapping explanations can be rightfully applied. Let us analyze a few examples:

1. The *Tostines mystery: Does Tostines sell more because it is always fresh and crunchy, or is it always fresh and crunchy because it sells more?*

This slogan was used at a very successful marketing campaign, that launched the relatively unknown brand Tostines, from Nestlé, to a leading position in the Brazilian market of biscuits, crackers and cookies. The expression *Tostines mystery* became idiomatic in Brazilian Portuguese, playing a role similar to that of the expression bootstrapping in English.

2. The C computer language and the UNIX operating system: Perhaps the most successful and influential computer language ever designed, C was conceived having boot-strapping in mind. The core language is powerful but spartan. Many capabilities that are an integral part of other programming languages are provided by functions in external standard libraries, including all device dependent operations such as input-output, string and file manipulation, mathematical computations, etc. C was part of a larger project to write UNIX as a portable operating system. In order to have UNIX and all of its goodies into a new machine (device drivers should already be there), we only have to translate the assembly code for a core C compiler, compile a full C compiler, compile the entire UNIX system, compile all the application programs we want, and voilà, we are done. Bootstrapping, as a technological approach, is of fundamental importance for the computer industry as it allows the development of evermore powerful software and the rapid substitution of hardware.

3. The Virtuous cycle of open source software: An initial or starting code contri-bution is made available at an *open source code repository*. *Developer communities* can use the resources at the repository according to the established open source license. De-velopers create software or application programs according to their respective business models, affected by the open source license agreements and the repository governance policy. The use of existing *software* motivates new applications or extensions to the ex-isting ones, generating the development of new programs and new contributions to the open source repository. Code contributions to the repository are filtered by a *controlling committee* according to a governance model. The full development cycle works using the highlighted elements as catalysts, and is fuelled by the work of self-interested individuals acting according to their own motivations, see Heiss (2007).

4. The Bethe-Weizsäcker main catalytic cycle (CNO-I):

$$^{12}_{6}\text{C} + ^{1}_{1}\text{H} \rightarrow ^{13}_{7}\text{N} + \gamma + 1.95\text{MeV}; \quad ^{13}_{7}\text{N} \rightarrow ^{13}_{6}\text{C} + e^{+} + \nu + 2.22\text{MeV};$$
$$^{13}_{6}\text{C} + ^{1}_{1}\text{H} \rightarrow ^{14}_{7}\text{N} + \gamma + 7.54\text{MeV}; \quad ^{14}_{7}\text{N} + ^{1}_{1}\text{H} \rightarrow ^{15}_{8}\text{O} + \gamma + 7.35\text{MeV};$$
$$^{15}_{8}\text{O} \rightarrow ^{15}_{7}\text{N} + e^{+} + \nu + 2.75\text{MeV}; \quad ^{15}_{7}\text{N} + ^{1}_{1}\text{H} \rightarrow ^{12}_{6}\text{C} + ^{4}_{2}\text{He} + 4.96\text{MeV}.$$
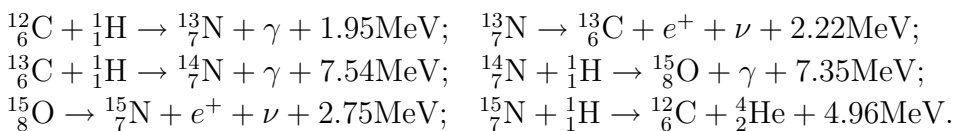
This example presents the nuclear synthesis of one atom of Helium from four atoms of Hydrogen. Carbon, Nitrogen and Oxygen act as catalysts in this cyclic reaction, that also produces gamma rays, positrons and neutrinos. Note that the Carbon-12 atom used in the first reaction is regenerated at the last one. The CNO nuclear fusion cycle is the main source of energy in stars with mass twice as large or more than that of the sun. We have included this example from nuclear physics in order to stress the fact that catalytic cycles play an important role in phenomena occurring in spatial and temporal scales which are much smaller than those typical of chemistry or biology, where some of the readers may find them more familiar.

5. RNA and DNA replication: DNA and RNA duplication, translation, and copying may, in general, be considered the core cycle of life, since it is the central cycle of biological

reproduction. Although even a simple description of this process is far too complex to be included in this book, its worth noting that RNA and DNA copy mechanisms rely on many enzymes and auxiliary structures, which are only available because they themselves are synthesized or regenerated in the living cell of other, also very complex, cyclical networks.

Examples 4 and 5 are taken from Eigen (1977). Examples 3 and 5 are, in Manfred Eigen's nomenclature, hypercycles. Eigen defines an *autocatalytic cycle* as a (chemical) reaction cycle that, using additional resources available in its environment, produces an excess of one or more of its own reactants. A *hypercycle* is an autocatalytic reaction of second or higher order, that is, an autocatalytic cycle connecting autocatalytic units. In a more general context, a hypercycle indicates self-reproduction of second or higher order, that is, a second or higher order cyclic production network including lower order self-replicative units. In the prototypical hypercycle architecture, a lower order self-replicative unit plays then a dual catalytic role: First, it has an auto-catalytic function in its own reproduction. Second, it acts like a catalyst promoting an intermediate step of the higher order cycle.

6.4.1   Bootstrapping Paradoxes

Let us now examine some ways in which the bootstrapping metaphor is wrongfully applied, that is, it is used to generate incongruent or inconsistent arguments, supposed to accommodate contradictory situations or to explain the existence of impossible processes. We will focus on four cases of historical interest and great epistemological importance.

Perpetua Mobile

Perhaps the best known paradox related to the bootstraping metaphor is connected to a class of examples known as Perpetuum Mobile machines. These machines are supposed to operate forever without any external help or even to produce some useful energy output. Unfortunately, perpetual mobiles are only wishful thinking, since the existence of such a machine would violate the first, second and third laws of thermodynamics. These are essentially "no free lunch" principles, formulated as inequalities for the flow (balance or transfer) of matter, energy and information in a general system, see Atkins (1984), Dugdale (1996) and Tarasov (1988).

Hypercyclical processes are not magical and must rely on energy, information (order or neg-entropy) and raw materials available at their environment. In fact, the use of external sources of energy and information is so important, that it entails the definition of metabolism used in Eigen (1977):

> Metabolism: (The process) can become effective only for intermediate states which are formed from energy-rich precursors and which are degraded to some

energy-deficient waste. The ability of the system to utilize the free energy and the matter required for this purpose is called metabolism. The necessity of maintaining the system far enough from equilibrium by a steady compensation of entropy production has been first clearly recognized by Erwin Schrödinger (1945).

The need for metabolism may come as a disappointment to professional wishful thinkers, engineers of perpeuum mobile machines, narcissistic philosophers and other anorexic designers. Nevertheless, it is important to realize that metabolic chains are in fact an integral part of the hypercycle concept. Hypercycles are built upon the possibility that the raw material that is supposed to be freely available in the environment for one autocatalytic reaction, may very well be the product of another catalytic cycle. Moreover, the same thermodynamic laws that prevent the existence of a perpeuum mobile, are fully compatible with a truly wonderful property of hypercycles, namely, their almost miraculous efficiency, as stated in Eigen (1977):

> Under the stated conditions, the product of the plain catalytic process will grow linearly with time, while the autocatalytic system will show exponential growth.

Evolutionary View

The exponential or hyperbolic (super-exponential) growth of processes based on autocatalytic cycles and hypercycles have profound evolutionary implications. Populations growing exponentially in environments with limited resources, or even with resources growing at a linear or polynomial rate, find themselves in the Maltusian conundrum of ever increasing individual or group competition for evermore scarce resources. In this setting, selection rules applied to a population of individuals struggling to survive and reproduce inexorably leads to an evolutive process. This qualitative argument goes back to Thomas Robert Malthus, Alfred Russel Wallace, and Charles Darwin, see Ingraham (1982) and Richards (1989).

Several alternative mathematical models for evolutive processes only confirm the soundness of the original Malthus-Wallace-Darwin argument. Eigen (1977, 1978a,b) analyses evolutionary processes on the basis of dynamical systems models using the language of ordinary differential equations. Stern (2008, ch.5) takes In Chapter 5 we take a completely different approach, analyzing evolutionary processes on the basis of stochastic optimization algorithms using the language of inhomogeneous Markov chains. For other possible approaches see Jantsch and Waddington (1976) and Jantsch (1980, 1981). It is remarkable however, that the qualitative conclusions of these distinct alternative analyses are in complete agreement.

The evolutionary view replaces a static scenario by a dynamic context. This replacement has the side effect of enhancing or amplifying most of the mirror-house illusions studied in this chapter. No wonder then, that the adoption of an evolutionary view requires from the observer a solid background on well founded scientific theories together with the firm domain of a logical and coherent epistemological framework in order to keep his or her balance and maintain straight judgment.

Building Blocks and Modularity

Another consequence of the analysis of evolutionary processes, using either the dynamical systems approach, see Eigen (1977, 1978a,b), or the stochastic optimization approach, see Chapter 5, is the spontaneous emergence of modular structures and hierarchical organization of complex systems.

A classic illustration of the need for modular organization is given by the Hora and Tempus parable of Simon (1996), see also Growney (1982). This is a parable about two watch makers, named Hora and Tempus, both of whom are respected manufacturers and, under ideal conditions, produce watches of similar quality and price. Each watch requires the assemblage of $n = 1000$ elementary pieces. However, while Hora uses a hierarchical modular design, Tempus does not. Hora builds each watch with 10 large blocks, each made of 10 small modules of 10 single parts each. Consequently, in order to make a watch, Hora needs to assemble $m = 111$ modules with $r = 10$ parts each, while Tempus needs to assemble only $m = 1$ module with $r = 1000$ parts. It takes either Hora or Tempus one minute to put a part in its proper place. Hence, while Tempus can assemble a watch in 1000 minutes, Hora can only do it in 1110 minutes. However both work in a noisy environment, being subject to interruptions (like receiving a telephone call). While placing a part an interruption occurrs with probability of $p = 0.01$. Partially assembled modules are unstable, braking down at an interruption. Under these conditions, the expected time to assemble a watch is

$$ \frac{m}{p} \left(\frac{1}{(1-p)^r} - 1 \right) \ . $$

Replacing p, m and r for the values in the parable, one finds that Hora's manufacturing process is a few thousand times more efficient then Tempus'. After this analysis, it is not difficult to understand why Tempus struggles while Hora prospers.

Closing yet another cycle, we thus came to the conclusion that the evolution of complex structures requires modular design. The need for modular organization is captured by the following dicta of Herbert Simon:

> *"Hierarchy, I shall argue, is one of the central structural schemes that the architect of complexity uses."* Simon (1996, p.184).

"The time required for the evolution of a complex form from simple elements depends critically on the number and distribution of potential intermediate stable subassemblies." Simon (1996, p.190).

"The claim is that the potential for rapid evolution exists in any complex system that consists of a set of subsystems, each operating nearly independently of the detailed process going on within the other subsystems, hence influenced mainly by the net inputs and outputs of the other subsystems. If the near-decomposability condition is met, the efficiency of one component (hence its contribution to organism fitness) does not depend on the detailed structure of other components." Simon (1996, p.193).

Standards and Once-Forever Choices

An important consequence of emerging modularity in evolutive processes is the recurrent commitment to once-forever choices and the spontaneous establishment of standards. This organizational side effect is responsible for mirror-house effects related to many misleading questions leading to philosophical dead-ends. Why do (almost all) nations use the French *meter, m,* as the standard unit of length, instead of the older Portuguese *vara* ($\approx 1.1m$) or the British *yard* ($\approx 0.9m$)? Why did the automotive industry select 87 octane as "regular" gasoline and settled for 12V as the standard voltage for vehicles? Why do we have chiral symmetry breaks, that is, why do we find only one specific type among two or more possible isomeric molecular forms in organic life? What is so special about the DNA - RNA genetic code that it is shared by all living organisms on planet earth?

In this mirror house we must accept that the deepest truth is often pretty shallow. Refusing to do so, insisting on extraction by forceps of more elaborate explanations, can take us seriously astray into foggy illusions, far away from clear reason and real understanding. Eigen (1977, p.541-542) makes the following comments:

> The Paradigm of Unity and Diversity in Evolution: Why do millions of species, plants and animals, exist, while there is only one basic molecular machinery of the cell, one universal genetic code and unique chiralities of the macromolecules?
>
> This code became finally established, not because it was the only alternative, but rather due to a peculiar 'once-forever' selection mechanism, which could start from any random assignment. Once-forever selection is a consequence of hypercyclic organization.

6.5   Squaring the Cycle

Ouroboros is a Greek name, *Ουροβορς οφις*, meaning the tail-devouring snake, see Eleazar

(1760) and Franz (1981). It is also an ancient alchemical symbol of self-reflexive or cyclic processes, of something perpetually re-creating itself. In modern cybernetics it is used as a representation of autopoiesis. The ourobouros is represented as a single, integral organism, the snake, whose head bites its own tail. This pictorial representation would not make much sense if the snake were cut into several pieces, yet, that is what may happen, if we are not careful, when trying to explain a cyclic process.

Let us illustrate this discussion with a schematic representation of the fiscal cycle of an idealized republic. This cycle is represented by a diagram similar to the one presented in section 7. This square diagram has four arrows pointing, respectively,
- Down: Citizens pay taxes to fulfill their duties;
- Left: Citizens elect a senate or a house of representatives;
- Up: The senate legislates fiscal policies; and
- Right: A revenue service enforces fiscal legislation.

Focusing on each one of the arrows we can speak, respectively, of
- Downward causation, whereby individuals comply with established social constraints;
- Upward causation, whereby the systems constraints are established and renewed;
- Leftward causation, whereby individuals (re)present new demands to the republic;
- Rightward causation, whereby the status quo is maintained, stabilized and enforced.

Each one of these causal relations is indeed helpful to understand the dynamic of our idealized republic. On the other hand, the omission of any single one of these relations breaks the cycle, and such an incomplete version of the schematic diagram would no longer explain a dynamical system.

The adjectives up and down capture our feelings as an individual living under social constraints (like costumes, moral rules, laws and regulations) that may (seem to) be overwhelming, while the adjectives left and right are late echoes of the seating arrangement in the French legislative assembly of 1791, with the conservatives, protecting aristocratic privileges of the ancien régime, seating on the right and the liberals, voicing the laissez-faire-laissez-passer slogans for free market capitalism, seating on the left. How to assign intuitive and meaningful positional or directional adjectives to links in a complex network is in general not so obvious. In fact, insisting on similar labeling practices is a common source of unnecessary confusion and misunderstanding. A practice that easily generates inappropriate interpretations is *polysemy*, the reuse of the same tags in different contexts. This is due to semantic contamination or spill over, that is, unwanted or unforeseen transfers of meaning, induced by polysemic overloading.

We can ask several questions concerning the relative importance of specific links in causal networks. For example: Can we or should we by any means establish precedences between the links in our diagram? Upward causes precede or have higher status then downward causes or vice versa? Rightward causes explain or have preponderance over leftward causes or vice versa? Do any of the possible answers imply a progressive or

revolutionary view? Do the opposite answers imply a conservative or reactionary view? The same questions can be asked with respect to a similar diagram for scientific production presented in section 7. Do any of the possible answers imply an empiricist or Aristotelic view? Do the opposite answers imply an idealistic or Platonic view?

To some degree these can be legitimate questions and consequently, to the same degree, motivate appropriate answers. Nevertheless, following the main goal of this chapter, namely, the exploration of mirror-house illusions, we want to stress that extreme forms of these questions often lead to ill posed problems. Therefore, extreme answers to the same questions often give an over simplified, one sided, biased, or distorted view of reality. The dangerous consequences of acceding to the temptation of having an appetizing ourobourus' slice for supper are depicted, in the field of psychology, by the following quotations from Efran (1990, p.99,47):

> Using language, any cycle can be broken into causes and purposes... Note that inventing purposes - and they are invented - is usually an exercise in creating tautologies. A description is turned into a purpose that is then asked to account for the description. [A typical example] starts with the defining characteristic of life, self-perpetuation, and states that it is the purpose for which the characteristic exists. Such circular renamings are not illegal, but they do not advance the cause (no pun intended). (p.99)
>
> For a living system there is a unity between product and process: In other words, the major line of work for a living system is creating more of itself.
>
> Autopoiesis in neither a promise nor a purpose - it is an organizational characteristic. This means that life lasts as long as it lasts. It doesn't come with guarantees. In contrast to what we are tempted to believe, people do not stay alive because of their strong survival instincts or because they have an important job to complete. They stay alive because their autopoietic organization happens to permit it. When the essentials of that organization are lost, a person's career comes to an end - he or she disintegrates. (p.47)

6.6   Emergence and Asymptotics

Asymptotic entities emerge in a model as a *law of large numbers*, that is, as a stable behavior of a quantity in the limiting case of model parameters corresponding to a system with very many (asymptotically infinite) components. The familiar mathematical notation used in these cases takes the form $\lim_{n\to\infty} g(n)$ or $\lim_{\epsilon\to 0} f(\epsilon)$. Typically, the underlying model describes a local interaction in a small or microscopic scale, while the resulting limit correspond to a global behavior in a large or macroscopic scale.

The paradigmatic examples in this class express the behavior of thermodynamic vari-

ables describing a system, such as volume, pressure and temperature of a gas, as asymptotic limits in statistical mechanics models for (infinitely) many interacting particles, like atoms or molecules, see Atkins (1984), Tarasov (1988). Other well known examples explain the behavior of macro-econometric relations among descriptive variables of efficient markets, like aggregated supply, demand, price and production, form micro-economic models for the interaction of individual agents, see Ingrao and Israel (1990). Even organic tissue movements in morphogenesis can be understood as the asymptotic limit of local cellular interactions at microscopic scale, as already mentioned in section 2. In this section we have chosen to examine some aspects of the collective behavior of flocks, schools and swarms, that can be easily visualized in a space and time scale directly assessible to our senses.

Large flocks of birds or schools of fish exhibit coordinated flight or swimming patterns and manifest collective reaction movements that give the impression that the collective entity has "a mind of its own". There are many explanations for why these animals swarm together. For example, they may do so in order to achieve:
- Better aerodynamic or hydrodynamic performance by flying or swimming in tight formation,
- More efficient detection of needed resources or dangerous threats by the pooling of many sensors;
- Increased reproductive and evolutive success by social selection rules; etc.
In this section, however, we will focus on another advantage:
- Reducing the risk of predation by evasive maneuvers.

The first point in the analysis of this example is to explain why it is a *valid example* of emergence, that is, to describe a possible local interaction model from which the global behavior emerges when the flock has a large number of individuals. We use the model programmed by Craig Reynolds (1987).

In 1986 I made a computer model of coordinated animal motion such as bird flocks and fish schools. It was based on three dimensional computational geometry of the sort normally used in computer animation or computer aided design. I called the generic simulated flocking creatures *boids*. The basic flocking model consists of three simple steering behaviors which describe how an individual boid maneuvers based on the positions and velocities its nearby flockmates:

Separation: steer to avoid crowding local flockmates

Alignment: steer towards the average heading of local flockmates

Cohesion: steer to move toward the average position of local flockmates

Each boid has direct access to the whole scene's geometric description, but flocking requires that it reacts only to flockmates within a certain small neighborhood around itself.

The second point is to explain why being part of a flock can reduce the risk of predation: Many predators, like a falcon hunting a sparrow, need to single out and focus on a chosen individual in order to strike accurately. However, the rapid change of relative positions of individuals in the flock makes it difficult to isolate a single individual as the designated target and follow it inside the moving flock. Computer simulation models show that this confusion effect greatly reduces the killing (success) rate in this kind of hunt.

The third point in our analysis is to contrast the hunting of single individuals, as analyzed in the previous paragraph, with other forms of predation based on the capture of the entire flock, or a large chunk of it. The focus of such alternative hunting techniques is, in the relative topology of the flock, not on local but on global variables describing the collective entity. For example, as explained in Diachok (2006) and Leighton et al. (2004, 2007), humpback whales collaborate using sophisticated strategies for hunting herring, including specific tactics for:

Detection: Whales use active sonar detection techniques, using specific frequencies that resonates with and are attenuated by the swim bladders of the herring. In this way, the whales can detect schools over long distances, and also measure its pertinent characteristics.

Steering: Some whales broadcast loud sounds below the herring school, driving them to the surface. Other whales blow a bubble-net around the school, spiraling in as the school rises. The herring is afraid of the loud sounds at the bottom, and also afraid of swimming through the bubble-net, and is thus forced into a dense pack at a compact killing zone near the surface.

Capture: Finally, the whales take turns at the killing zone, raising to the surface with their mouths wide open, catching hundreds of fish at a time or, so to speak, "biting of" large chunks of the school.

Finally, let us propose two short statements that can be distilled from our examples. They are going to carry us to the next section.

- Flocking makes it difficult for a predator to use *local tactics* tracking the trajectory of a single individual, consequently, for a hunter that focus on local variables it is *hard to know* what exactly is going on.

- On the other hand, the same collective behavior creates the opportunity for *global strategies* that track and manipulate the entire flock. These hunting technique may be very efficient, in which case, we can say that the hunters *know very well* what they are doing.

	Experiment				Theory

Operation-alization	$\Leftarrow$	Experiment design	$\Leftarrow$	Hypotheses formulation
$\Downarrow$				$\Uparrow$
Effects observation		True/False eigen-solution		Creative interpretation
$\Downarrow$				$\Uparrow$
Data acquisition	$\Rightarrow$	Mnemetic explanation	$\Rightarrow$	Statistical analysis

Sample space Parameter space
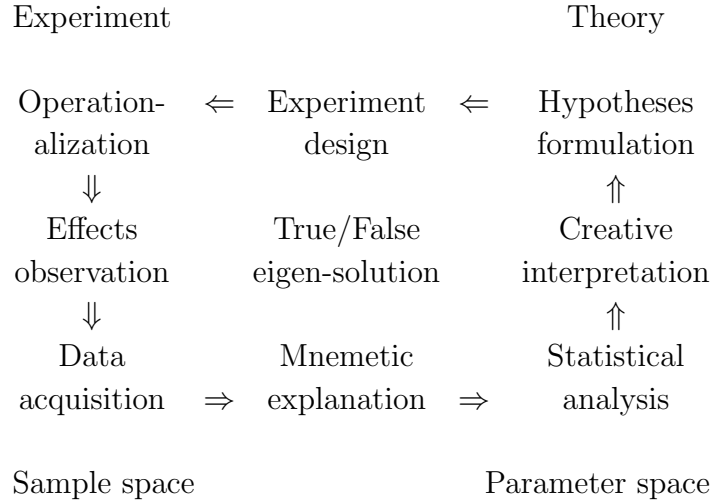
Figure 1: Scientific production diagram.

6.7 Constructive Ontologies

From the several examples mentioned in sections 2, 4 and 6, we can suspect that the emergence of properties, behaviors, organizational forms and other entities are the rule rather than the exception for many non-trivial systems. Hence it is natural to ask about the ontological status of such entities. Ontology is a term used in philosophy referring to a systematic account of *existence* or *reality*. In this section we analyze the ontological status of emergent entities according to the Cog-Con epistemological framework. The following paragraphs give a brief summary of this perspective, as well as some specific epistemological terms as they are used in the Cog-Con framework.

The interpretation of scientific knowledge as an eigensolution of a research process is part of a Cog-Con approach to epistemology. Figure 1 presents an idealized structure and dynamics of knowledge production. This diagram represents, on the Experiment side (left column) the laboratory or field operations of an empirical science, where experiments are designed and built, observable effects are generated and measured, and the experimental data bank is assembled. On the Theory side (right column), the diagram represents the theoretical work of statistical analysis, interpretation and (hopefully) understanding according to accepted patterns. If necessary, new hypotheses (including whole new theories) are formulated, motivating the design of new experiments. Theory and experiment constitute a double feed-back cycle making it clear that the design of experiments is guided by the existing theory and its interpretation, which, in turn, must be constantly checked, adapted or modified in order to cope with the observed experiments. The whole system constitutes an autopoietic unit.

The Cog-Con framework also includes the following definition of reality and some related terms:

1. Known (knowable) Object: An actual (potential) eigen-solution of a given system's interaction with its environment. In the sequel, we may use a somewhat more friendly terminology by simply using the term Object.

2. Objective (how, less, more): Degree of conformance of an object to the essential attributes of an eigen-solution (to be precise, stable, separable and composable).

3. Reality: A (maximal) set of objects, as recognized by a given system, when interacting with single objects or with compositions of objects in that set.

The Cog-Con framework assumes that an object is always observed by an observer, just like a living organism or a more abstract system, interacting with its environment. Therefore, this framework asserts that the manifestation of the corresponding eigen-solution and the properties of the object are respectively driven and specified by both the system and its environment. More concisely, Cog-Con sustains:

4. Idealism: The belief that a system's knowledge of an object is always dependent on the systems' autopoietic relations.

5. Realism: The belief that a system's knowledge of an object is always dependent on the environment's constraints.

Consequently, the Cog-Con perspective requires a fine equilibrium, called *Realistic or Objective Idealism. Solipsism or Skepticism* are symptoms of an epistemological analyses that looses the proper balance by putting too much weight on the idealistic side. Conversely, *Dogmatic Realism* is a symptom of an epistemological analyses that looses the proper balance by putting too much weight on the realistic side. Dogmatic realism has been, from the Cog-Con perspective, a very common (but mistaken) position in modern epistemology. Therefore, it is useful to have a specific expression, namely, *something in itself* to be used as a marker or label for such ill posed dogmatic statements. The method used to access something in itself is often described as: - Something that an observer would observe if the (same) observer did not exist, or - Something that an observer could observe if he made no observations, or - Something that an observer should observe in the environment without interacting with it (or disturbing it in any way), and many other equally senseless variations.

From the preceding considerations, it should become clear that, from the Cog-Con perspective, the ontological status of emergent entities can be perfectly fine, as long as these objects correspond to precise, stable, separable and composable eigen-solutions. However there is a long list of historical objections and complaints concerning such entities. The following quotations from Pihlstrom and El-Hani (2002) elaborate on this point.

> Emergent properties are not metaphysically real independently of our practices of inquiry but gain their ontological status from the practice-laden ontological commitments we make.

> [concerning] the issue of the ontological epistemological status of emergents ... we simply need to be careful in our recognition of emergent phenomena and continually ask the question of whether the pattern we see is more in our eye than the pattern we are claiming to see.
>
> Related to the supposed provisionality of emergents is the issue of their ontological status: Are emergent phenomena part of the real, authentic "furniture of the world", or are they merely a function of our epistemological, cognitive apparatus with its ever-ready mechanism of projecting patterns on to the world?

From the summary of the Cog-Con epistemological framework presented above we conclude that, from this perspective, we have to agree with the first observations, and consider the last question as an ill posed problem.

Another set of historical issues concerning the ontological status of emergents relates to our ways of understanding them. For some authors, "real" emergent entities must be genuinely "new", in the sense of being unanalyzable or unexplainable. For such authors, understanding is a mortal sin that threatens the very existence on an entity, that is, understanding undermines their ontological status. Hence, according to these authors, the most real of entities should always be somewhat mysterious. Vieira and El-Hani (2009, p.105), analyze this position:

> A systemic property P of a system S will be irreducible if it does not follow, even in principle, from the behavior of the system's parts that S has property P.
>
> If a phenomenon is emergent by reasons of being unanalyzable, it will be an unexplainable, brute fact, or, to use Alexander's (1920/1979) words, something to be accepted with natural piety. We will not be able to predict or explain it, even if we know its basal conditions.
>
> In our view, if the understanding of the irreducibility of emergent properties is limited to this rather strong sense, we may lose from sight the usefulness of the concept... Indeed, claims about emergence turn out to be so strong, if interpreted exclusively in accordance with this mode of irreducibility, that they are likely to be false, at least in the domain of natural science (with are our primary interest in this chapter).

We fully agree with Vieira and El-Hani in rejecting unanalyzability or unexplainability as conditions for the "real existence" of emergent entities. As expected, the Cog-Con framework does not punish understanding, far from it. In Chapter 4, the Cog-Con perspective for the meaning of objects in a specific reality is given by their interrelation in a network of causal nexus, explaining *why* the corresponding eigen-solutions manifest

themselves the way they do. Such explanations include, specially in modern science, the symbolic derivation of scientific hypotheses from general scientific laws, the formulation of new laws in an existing theory, and even the conception of new theories, as well as their general understanding based on accepted metaphysical principles. In the Cog-Con perspective, the understanding of an entity can only strengthen its ontological status, embedding it even deeper in the system's life, endowing it with even wider connections in the web of concepts, revealing more of its links with the great chain of being!

6.8 Distinctions and Probability

In the last two sections we have analyzed emergent objects and their properties. In many of the examples used in our discussions, probability mechanisms where at the core of the emergence process. In this section, other ways in which probability mechanisms can generate complex or non-trivial structures will be presented. This section is also dedicated to the study of the ontological status of probability, and the role played by explanations given by probabilistic mechanisms and stochastic causal relations. We begin our discussion examining the concept of mixed strategies in game theory, due to von Neumann and Morgenstern.

Let us consider the *matching pennies* game, played by Odd and Even. Each of the players has to show, simultaneously, a bit (0 or 1). If both bits agree (i.e., 00 or 11), Odd wins. If both bits disagree (i.e., 01 or 10), Even wins. Both players only have two pure or deterministic strategies available from which to choose: s_0 - show a 0, or s_1 - show a 1.

A *solution, equilibrium* or *saddlepoint* of a game is a set of strategies that leaves each player at a local optimum, that is, a point at which each player, having full knowledge of all the other players' strategies at that equilibrium point, has nothing to gain by unilaterally changing his own strategy. It is easy to see that, considering only the two deterministic strategies, the game of matching pennies has no equilibrium point. If Odd knows the strategy chosen by Even, he can just take the same strategy and win the game. In the same way, Even can take the opposite choice of Odd's, and win the game.

Let us now expand the set of strategies available to each player considering *mixed* or *randomized* strategies, where each player picks among the pure strategies according to a set of probabilities he specifies. We assume that a proper randomization device, like a dice, a roulette or a computer with a random number generator program, is available. In the example at hand, Even and Odd can each specify a probability, respectively, pe and po, for showing a 1, and $qe = 1 - pe$ and $qo = 1 - po$, for showing a 0. It is easy to check that $pe = po = 1/2$ is a solution to this game.

Oskar Morgenstern (2008, p.270) makes the following comments about the philosophical significance of mixed strategies:

It is necessary to examine the significance of the use of mixed strategies since they involve probabilities in situations in which 'rational' behavior is looked for. It seems difficult, at first, to accept the idea that 'rationality' - which appears to demand a clear, definite plan, a deterministic resolution - should be achieved by the use of probabilistic devices. Yet precisely such is the case.

In games of chance the task is to determine and then to evaluate probabilities inherent in the game; in games of strategy we introduce probability in order to obtain the optimal choice of strategy. This is philosophically of some interest.

The role played by mixed strategies can be explained, at least in part, by convex geometry. A *convex combination* of two points, p_0 and p_1, is a point lying on the line segment joining them, that is, a point of the form $p(\lambda) = (1 - \lambda)p_0 + \lambda p_1$, $0 \leq \lambda \leq 1$. A *convex set* is a set that contains all convex combinations of its points. The *extreme points* of a convex set are those that can not be expressed as (non-trivial) convex combinations of other points in the set. A function $f(x)$ is convex if its epigraph, epi(f) - the set of all point above the graph of $f(x)$, is convex. A *convex optimization problem* consists of minimizing a convex function over a convex region. The properties of convex geometry warrant that a convex optimization problem has an optimal solution, i.e. a minimum, $f(x^*)$. Moreover, the minimum argument, x^*, is easy to compute using a procedure such as the *steepest descent algorithm*, that can be informally stated as follows: Place a particle at some point over the graph of $f(x)$, and let it "roll down the hill" to the bottom of the valley, until it finds its lowest point at x^*, see Luenberger (1984) and Minoux (1986).

In the matching pennies game, let us consider a convex combination of the two pure strategies, that is, a strategy of the form $s(\lambda) = (1-\lambda)s_0 + \lambda s_1$, $0 \leq \lambda \leq 1$. Since the pure strategies form a discrete set, such continuous combination of pure strategies is not even well defined, except for the trivial extreme cases, $\lambda = 0$ or $\lambda = 1$. The introduction of randomization gives a coherent definition for convex combinations of existing strategies and, in so doing, it expands the set of available (mixed) strategies to a convex set where pure strategies become extreme points. In this setting, a game equilibrium point can be characterized as the solution of a convex optimization problem. Therefore, such an equilibrium point exists and is easy to compute. This is one way of having a geometric understanding of von Neumann and Morgenstein theorems, as well as to subsequent extensions in game theory due to John F. Nash, see Bonassi et al. (2009), Mesterton-Gibbons (1992) and Thomas (1986).

The matching pennies example poses a $\delta\iota\lambda\eta\mu\mu\alpha$, dilemma - a problem offering two possibilities, none of which is acceptable. The conceptual dichotomy created by constraining the players to only two deterministic strategies creates an ambush. Caught in this ambush, both players would be trapped, forever changing their minds between extreme

options. Randomization expands the universe of available possibilities and, in so doing, allows the players to escape the perpetual flip-flopping at this discrete logic decision trap. In section 8.2, we extrapolate this example and generalize these conclusions. However, before proceeding in this direction, we shall analyze, in the next section, some objections to the concepts of probability, statistics and randomization posed by George Spencer-Brown, a philosopher of great influence in the field of radical constructivism.

6.8.1   Spencer-Brown, Probability and Statistics

Spencer-Brown (1953, 1957) analyzed some apparent paradoxes involving the concept of randomness, and concluded that the language of probability and statistics is inappropriate for the practice of scientific inference. In subsequent work, Spencer Brown (1969) reformulates classical logic using only a generalized *nor* operator (marked *not-and* unmarked *or*), that he represents à la mode of Charles Saunders Peirce or John Venn, using a graphical boundary or distinction mark, see Edwards (2004), Kauffmann (2001, 2003), Meguire (2003), Peirce (1880), Sheffer (1913). Making distinctions is, according to Spencer-Brown, the basic (if not the only) operation of human knowledge, an idea that has either influenced or been directly explored by several authors in the radical constructivist movement. Some typical arguments used by Spencer-Brown in his rejection of probability and statistics are given in the next quotations from Spencer-Brown (1957, p.66,105,113):

> We have found so far that the concept of probability used in statistical science is meaningless in its own terms; but we have found also that, however meaningful it might have been, its meaningfulness would nevertheless have remained fruitless because of the impossibility of gaining information from experimental results, however significant This final paradox, in some ways the most beautiful, I shall call the Experimental Paradox (p.66).
>
> The essence of randomness has been taken to be absence of pattern. But has not hitherto been faced is that the absence of one pattern logically demands the presence of another. It is a mathematical contradiction to say that a series has no pattern; the most we can say is that it has no pattern that anyone is likely to look for. The concept of randomness bears meaning only in relation to the observer: If two observers habitually look for different kinds of pattern they are bound to disagree upon the series which they call random. (p.105).

In Section G.1 I carefully explain why I disagree with Spencer-Brown's analysis of probability and statistics. In some of my arguments I dissent from Spencer-Brown's interpretation of measures of order-disorder in sequential signals. These arguments are based on information theory and the notion of entropy. Atkins (1984), Attneave (1959), Dugdale (1996), Krippendorff (1986) and Tarasov (1988) review some of the basic concepts

in this area using only elementary mathematics. For more advanced works see Kapur (1989), Rissanen (1989) and Wallace (2005). Several authors concur, at least in part, with my opinion about Sencer-Brown's analysis of probability and statistics, see Flew (1959), Falk and Konold (1997), Good (1958) and Mundle (1959).

I also disapprove some of Spencer Brown's proposed methodologies to detect "relevant" event sequences, that is, his criteria to "mark distinct patterns" in empirical observations. My objections have a lot in common with the standard caveats against *ex post facto* "fishing expeditions" for interesting outcomes, or simple *post hoc* "sub-group analysis" in experimental data banks. This kind of retroactive or retrospective data analyses is considered a questionable statistical practice, and pointed as the culprit of many misconceived studies, misleading arguments and mistaken conclusions. The literature of statistical methodology for clinical trials has been particularly active in warning against this kind of practice, see Tribble (2008) and Wang (2007) for two interesting papers addressing this specific issue and published in high impact medicine journals less than a year before I began writing this chapter. When consulting for pharmaceutical companies or advising in the design of statistical experiments, I often find it useful to quote Conan Doyle's Sherlock Holmes, in The Adventure of Wisteria Lodge:

> Still, it is an error to argue in front of your data. You find yourself insensibly twisting them around to fit your theories.

Finally, I am suspicious or skeptical about some of the intended applications of Spencer-Brown's research program, including the use of extrasensory empathic perception for coded message communication, exercises on object manipulation using paranormal powers, etc. Unable to reconcile his psychic research program with statistical science, Spencer-Brown had no regrets in disqualifying the later, as he clearly stated at the prestigious scientific journal *Nature*, Spence-Brown (1953b, p.594-595):

> [On telepathy:] Taking the psychical research data (that is, the residuum when fraud and incompetence are excluded), I tried to show that these now threw more doubt upon existing pre-suppositions in the theory of probability than in the theory of communication.

> [On psychokinesis:] If such an 'agency' could thus 'upset' a process of randomizing, then all our conclusions drawn through the statistical tests of significance would be equally affected, including the the conclusions about the 'psychokinesis' experiments themselves. (How are the target numbers for the die throws to be randomly chosen? By more die throws?) To speak of an 'agency' which can 'upset' any process of randomization in an uncontrollable manner is logically equivalent to speaking of an inadequacy in the theoretical model for empirical randomness, like the luminiferous ether of an earlier con-

troversy, becomes, with the obsolescence of the calculus in which it occurs, a superfluous term.

Sencer-Brown's (1953, 1957) conclusions, including his analysis of probability, were considered to be controversial (if not unreasonable or extravagant) even by his own colleagues at the Society of Psychical Research, see Scott (1958), and Soal (1953). It seems that current research in this area, even if not free (or afraid) of criticism, has abandoned the path of naïve confrontation with statistical science, see Atmanspacher (2005) and Ehm (2005). For additional comments, see Henning (2006), Kaptchuk and Kerr (2004), Utts (1991), and Wassermann (1955).

Curiously, Charles Saunders Peirce and his student Joseph Jastrow, who introduced the idea of randomization in statistical trials, struggled with some of the very same dilemmas faced by Spencer-Brown, namely, the eventual detection of distinct patterns or seemingly ordered (sub)strings in a long random sequence. Peirce and Jastrow did not have at their disposal the heavy mathematical artillery I have cited in the previous paragraphs. Nevertheless, like experienced explorers that when traveling in the desert are not lured by the mirage of a misplaced oasis, these intrepid pioneers were able to avoid the conceptual pitfalls that lead Spencer-Brown so far astray. For more details see Bonassi et al. (2008), Dehue (1997), Hacking (1988), and Peirce and Jastrow (1885).

As stated in the introduction, the Cog-Con framework is supported by the FBST, a formalism based on a non-decision theoretic form of Bayesian statistics. The FBST was conceived as a tool for validating objective knowledge and, in this role, it can be easily integrated to the Cog-Con epistemological framework in the practice of scientific research. Contrasting our distinct views of cognitive constructivism, it is not at all surprising that I have come to conclusions concerning the use of probability and statistics, and also to the relation between probability and logic, that are fundamentally different from those of Spencer-Brown.

6.8.2   Overcoming Dilemmas and Conceptual Dichotomies

As stated by William James, our ways of understanding require us to split reality with conceptual distinctions. The non-trivial consequences of the resulting dichotomies are captured, almost poetically, by James (1909, Lecture VI) in the following passage from *A Pluralistic Universe*:

> The essence of life is its continuously changing character; but our concepts are all discontinuous and fixed, and the only mode of making them coincide with life is by arbitrarily supposing positions of arrest therein. With such arrests our concepts may be made congruent. But these concepts are not parts of reality, not real positions taken by it, but suppositions rather, notes

taken by ourselves, and you can no more dip up the substance of reality with them than you can dip up water with a net, however finely meshed.

When we conceptualize, we cut out and fix, and exclude everything but what we have fixed. A concept means a that-and-no-other. Conceptually, time excludes space; motion and rest exclude each other; approach excludes contact; presence excludes absence; unity excludes plurality; independence excludes relativity; 'mine' excludes 'yours'; this connection excludes that connection - and so on indefinitely; whereas in the real concrete sensible flux of life experiences compenetrate each other so that it is not easy to know just what is excluded and what not...

The conception of the first half of the interval between Achilles and the tortoise excludes that of the last half, and the mathematical necessity of traversing it separately before the last half is traversed stands permanently in the way of the last half ever being traversed. Meanwhile the living Achilles... asks no leave of logic.

Sure enough, our way of understanding requires us to make those conceptual distinctions that are most adequate (or adequate enough) for a given reality domain. However, the concepts that are appropriate to analyze reality at a given level, scale or granularity, may not be adequate at the next level, that may be lower or higher, larger or smaller, coarser or finer. How then can we avoid being trapped by such distinctions? How can we overcome the distinctions made at one level in order to be able to reach the next, and still maintain a coherent or congruent view of the universe?

The Cog-Con endeavor requires languages and mechanisms to overcome the limitations of conceptual distinctions and, at the same time, enable us to coherently build new concepts that can be used at the next or new domains. Of course, as in all scientific research, the goal of the new conceptual constructs is to entail theories and hypotheses providing objective knowledge (in its proper domain), and the success of the new theories must be judged pragmatically according to this goal. I claim that statistical models and their corresponding probabilistic mechanisms, have been, in the history of modern science, among the most successful tools for accomplishing the task at hand. In Chapter 5, for example, we have shown in some detail how probabilistic reasoning can be used:

- In quantum mechanics, using the language of Fourier series and transforms, to overcome the dilemmas posed by a physical theory using concepts and laws coming from two distinct and seemingly incompatible categories: The mechanics of discrete particles and wave propagation in continuous media or fields.

- In stochastic optimization, using the language of inhomogeneous Markov chains, to overcome the dilemmas generated by dynamic populations of individuals with the need of reliable reproduction, hierarchical organization, and stable building blocks versus the need of creative evolution with innovative change or mutation.

In an empirical science, from a pragmatical perspective, probability reasoning seems to be an efficient tool for overcoming artificial dichotomies, allowing us to bridge the gaps created by our own conceptual distinctions. Such probabilistic models have been able to generate new eigen-solutions with very good characteristics, that is, eigen-solutions that are very objective (precise, stable, separable and composable). These new objects can then be used as stepping stones or building blocks for the construction of new, higher order theories. In this context, we thus assign, coherently with the Cog-Con epistemological framework, a high ontological status to probabilistic concepts and causation mechanisms, that is, we use a notion of probability that has a distinctively *objective* character.

6.9   Final Remarks and Future Research

The objective of this chapter was to use the Cog-Con framework for the understanding of massively complex and non-trivial systems. We have analyzed several forms of system complexity, several ways in which systems become non-trivial, and some interesting consequences, side effects and paradoxes generated by such non-triviality. How can we call the massive non-triviality found in nature? I call it *The Living and Intelligent Universe.* I could also call it *Deus sive natura* or, according to Einstein,

> *Spinoza's God, a God who reveals himself in the orderly harmony of what exists...*

In future research we would like to extend the use of the same Cog-Con framework to the analysis of the ethical conduct of agents that are conscious and (to some degree) self-aware. The definition of ethics given by Russell (1999, p.67), reads:

> *The problem of Ethics is to produce a harmony and self-consistency in conduct, but mere self-consistency within the limits of the individual might be attained in many ways. There must therefore, to make the solution definite, be a universal harmony; my conduct must bring satisfaction not merely to myself, but to all whom it affects, so far as that is possible.*

Hence, in this setting, such a research program should be concerned with the understanding and evaluation of choices and decisions made by agents, acting in a system in which they belong. Such an analysis should provide criteria for addressing the coherence and consistency of the behavior of such agents, including the direct, indirect and reflexive consequences of their actions. Moreover, since we consider conscious agents, their values, beliefs and ideas should also be included in the proposed models. The importance of pursuing this line of research, and also the inherent difficulties of this task, are summarized by Eigen (1992, p.126):

But long and difficult will be our ascent from the lowest landing up to the topmost level of life, the level of self-awareness: our continued ascent from man to humanity.

Goertzel (2008) points to generalizations of standard probabilistic and logical formalisms, and urges us to explore further connections between them, see for example Borges and Stern (2007), Caticha (2008), Costa (1986, 1993), Jaynes (1990), Stern (2004) and Youssef (1994, 1995). I am fully convinced that this path of cross fertilization between probability and logic is another important field for future research.

Epilog

In six chapters and ten appendices, we have presented our case in defense of a constructivist epistemological framework and the use of compatible statistical theory and inference tools. In this final remarks, we shall try to wrap up, as concisely as possible, the reasons for adopting the constructivist world-view.

The basic metaphor of decision theory is the maximization of a gambler's expected fortune, according to his own subjective utility, prior beliefs an learned experiences. This metaphor has proven to be very useful, leading the development of Bayesian statistics since its XX-th century revival, rooted on the work of de Finetti, Savage and others.

The basic metaphor presented in this text, as a foundation for cognitive constructivism, is that of an eigen-solution, and the verification of its objective epistemic status. The FBST is the cornerstone of a set of statistical tolls conceived to assess the epistemic value of such eigen-solutions, according to their four essential attributes, namely, sharpness, stability, separability and composability. We believe that this alternative perspective, complementary to the one offered by decision theory, can provide powerful insights and make pertinent contributions in the context of scientific research.

To fulfill our promise of concision, we finish here this summer course / tutorial. We sincerelly thank the readers for their attention and welcome their constructive comments. May the blessings of the three holy knights in Figure J.2-4 protect and guide you in your way. Fair well and goodbye!

"E aquela era a hora do mais tarde.
O céu vem abaixando. Narrei ao senhor.
No que narrei, o senhor talvez até ache,
mais do que eu, a minha verdade.
Fim que foi."

And it was already the time of later on,
the time of sun-down. My story I have told,
my lord, so that you may find, perhaps even
better than me, the truth I wanted to tell.
The End (that already was).

"Vivendo, se aprende; mas o que se aprende,
mais, é só a fazer outras maiores perguntas."

Living one learns, but what one learns,
is only how to ask even bigger questions.

João Guimarães Rosa (1908-1967).
Grande Sertão: Veredas.

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Appendix A

FBST Review

"(A) man's logical method should be loved and reverenced as his bride, whom he has chosen from all the world. He need not contemn the others; on the contrary, he may honor them deeply, and in doing so he honors her more. But she is the one that he has chosen, and he knows that he was right in making that choice."

C.S.Peirce (1839 - 1914),
The Fixation of Belief (1877).

"Make everything as simple as possible, but not simpler."

Albert Einstein (1879 - 1955).

A.1 Introduction

The FBST was specially designed to give a measure of the *epistemic value* of a sharp statistical hypothesis H, given the observations, that is, to give a measure of the *value of evidence* in support of H given by the observations. This measure is given by the support function ev(H), the FBST *e-value*. Furthermore the e-value has many necessary or desirable properties for a statistical support function, such as:

(I) Give an intuitive and simple measure of significance for the hypothesis in test, ideally, a *probability* defined directly in the original or *natural parameter space*.

(II) Have an intrinsically geometric definition, independent of any non-geometric aspect, like the particular parameterization of the (manifold representing the) null hypothesis being tested, or the particular coordinate system chosen for the parameter space, i.e., be an *invariant* procedure.

(III) Give a measure of significance that is smooth, i.e. *continuous and differentiable,*

245

on the hypothesis parameters and sample statistics, under appropriate regularity conditions for the model.

(IV) Obey the *likelihood principle* , i.e., the information gathered from observations should be represented by, and only by, the likelihood function, see Berger and Wolpert (1988), Pawitan (2001, ch.7) and Wechsler et al. (2008).

(V) Require *no ad hoc artifice* like assigning a positive prior probability to zero measure sets, or setting an arbitrary initial belief ratio between hypotheses.

(VI) Be a *possibilistic* support function, where the support of a logical disjunction is the maximum support among the support of the disjuncts.

(VII) Be able to provide a *consistent* test for a given sharp hypothesis.

(VIII) Be able to provide *compositionality* operations in complex models.

(IX) Be an *exact* procedure, i.e., make no use of "large sample" asymptotic approximations when computing the *e*-value.

(X) Allow the incorporation of previous experience or expert's opinion via (subjective) *prior distributions*.

The objective of this section is to provide a very short review of the FBST theoretical framework, summarizing the most important statistical properties of its support function, the *e*-value. It also summarizes the logical (algebraic) properties of the *e*-value, and its relations to other classical support calculi, including possibilistic calculus and logic, paraconsistent and classical. Further details, demonstrations of theoretical properties, comparison with other statistical tests for sharp hypotheses, and an extensive list of references can be found in the author's previous papers.

A.2   The Epistemic *e*-values

Let $\theta \in \Theta \subseteq R^p$ be a vector parameter of interest, and $L(\theta \,|\, x)$ be the likelihood associated to the observed data x, a standard statistical model. Under the Bayesian paradigm the posterior density, $p_n(\theta)$, is proportional to the product of the likelihood and a prior density,

$$p_n(\theta) \propto L(\theta \,|\, X)\, p_0(\theta).$$

The (null) hypothesis H states that the parameter lies in the null set, defined by inequality and equality constraints given by vector functions g and h in the parameter space.

$$\Theta_H = \{\theta \in \Theta \,|\, g(\theta) \leq \mathbf{0} \wedge h(\theta) = \mathbf{0}\}$$

From now on, we use a relaxed notation, writing H instead of Θ_H. We are particularly interested in sharp (precise) hypotheses, i.e., those in which there is at least one equality constraint and hence, $\dim(H) < \dim(\Theta)$.

The FBST defines ev(H), the *e*-value supporting (in favor of) the hypothesis H, and $\overline{\text{ev}}(H)$, the *e*-value against H, as

$$s(\theta) = \frac{p_n(\theta)}{r(\theta)} \ , \quad s^* = s(\theta^*) = \sup_{\theta \in H} s(\theta) \ , \quad \widehat{s} = s(\widehat{\theta}) = \sup_{\theta \in \Theta} s(\theta) \ ,$$

$$T(v) = \{\theta \in \Theta \,|\, s(\theta) \le v\} \ , \quad W(v) = \int_{T(v)} p_n(\theta) \, d\theta \ , \quad \text{ev}(H) = W(s^*) \ ,$$

$$\overline{T}(v) = \Theta - T(v) \ , \quad \overline{W}(v) = 1 - W(v) \ , \quad \overline{\text{ev}}(H) = \overline{W}(s^*) = 1 - \text{ev}(H) \ .$$

The function $s(\theta)$ is known as the posterior surprise relative to a given reference density, $r(\theta)$. $W(v)$ is the cumulative surprise distribution. The surprise function was used, among other statisticians, by Good [23], Evans [16] and Royall [48]. Its role in the FBST is to make ev(H) explicitly invariant under suitable transformations on the coordinate system of the parameter space, see next section.

The tangential (to the hypothesis) set $\overline{T} = \overline{T}(s^*)$, is a Highest Relative Surprise Set (HRSS). It contains the points of the parameter space with higher surprise, relative to the reference density, than any point in the null set H. When $r(\theta) \propto 1$, the possibly improper uniform density, $\overline{T}$ is the Posterior's Highest Density Probability Set (HDPS) tangential to the null set H. Small values of $\overline{\text{ev}}(H)$ indicate that the hypothesis traverses high density regions, favoring the hypothesis.

Notice that, in the FBST definition, there is an optimization step and an integration step. The optimization step follows a typical *maximum probability* argument, according to which, "a system is best represented by its highest probability realization". The integration step extracts information from the system as a probability weighted average. Many inference procedures of classical statistics rely basically on maximization operations, while many inference procedures of Bayesian statistics rely on integration (or marginalization) operations. In order to achieve all its desired properies, the FBST procedure has to use both, as explained in this appendix.

The evidence value, defined above, has a simple and intuitive geometric characterization. We now illustrate the above definitions with two simple but non-trivial examples. These two exemples are easy to visualize, since they have a two dimensional parameter space, and are also non-trivial, in the sense that they have a non-linear hypothesis.

Coefficient of Variation

The Coefficient of Variation (CV) of a random variable X is defined as the ratio $CV(X) = \sigma(X)/E(X)$, i.e. the ratio of its standard deviation to its mean. Let X be a normal random variable, with unknown mean and variance. We want to compute the evidence value supporting the hypothesis that the coefficient of variation of X is equal to a given

constant,

$$X \sim N(\beta, \sigma) \quad , \quad H : \ \sigma/\beta = c$$

The conjugate family for this problem is the family of bivariate distributions, where the conditional distribution of the mean β, for a fixed precision $\rho = 1/\sigma^2$, is normal, and the marginal distribution of the precision ρ is gamma, DeGroot (1970). Using the standard improper priors, uniform on $]-\infty, +\infty[$ for β, and $1/\rho$ on $]0, +\infty[$ for ρ, we get the posterior joint distribution for β and ρ:

$$p_n(\beta, \rho \,|\, x) \propto \sqrt{\rho} \, exp(-n\rho(\beta - \bar{x})^2/2) \, \rho^{\frac{n-2}{2}} exp(-\rho s n/2)$$

$$x = [x_1 \ldots x_n] \ , \bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i \ , \ s = \sum_{i=1}^{n} (x_i - \bar{x})^2$$
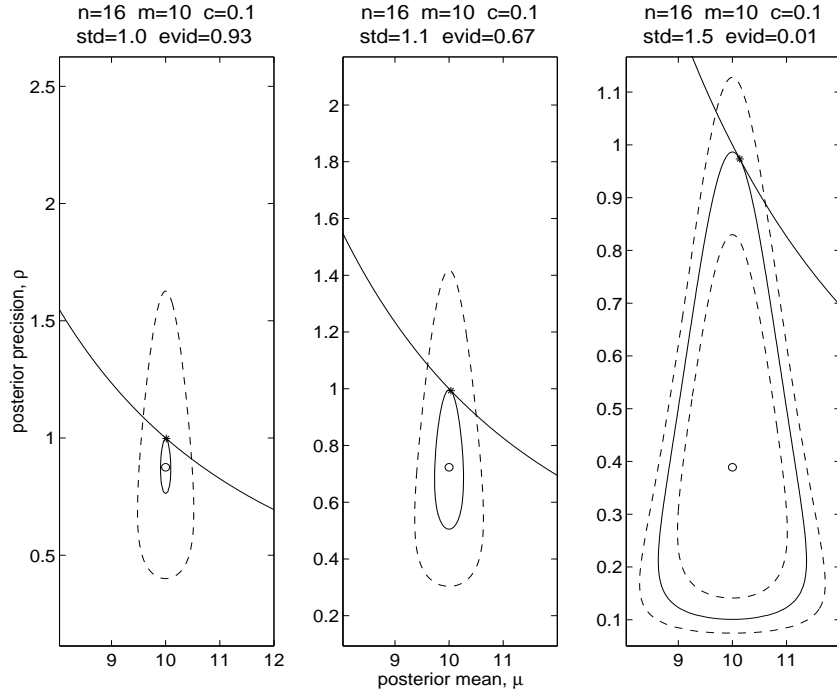
Figure A.1: FBST for H: CV=0.1

Figure A.1 shows the null set H, the tangential HRSS $\overline{T}$, and the points of constrained and unconstrained maxima, θ^* and $\widehat{\theta}$, for testing the hypothesis at hand with the following numerical example: $CV = 0.1$ with 3 samples of size $n = 16$, mean $\bar{x} = 10$ and standard deviations $std = 1.0$, $std = 1.1$ and $std = 1.5$. We can see the tangent set expanding as the sample standard deviation over mean ratio gets farther away from the coefficient of variation being tested, $CV(X) = \sigma(X)/E(X) = 0.1$. In this example we use the standard improper prior density and the uniform reference density. In the first plot, the sample

standard deviation over mean ratio equals the coefficient of variation tested. Nevertheless, the evidence against the null hypothesis is not zero; this is because of the non uniform prior. In order to test other hypotheses we only have to change the constraint(s) passed to the optimizer. Constraints for the hypothesis $\beta = c$ and $\sigma = c$ would be represented by, respectively, vertical and horizontal lines. All the details for these and other simple examples, as well as comparisons with standard frequentist and Bayesian tests, can be found in Irony et al. (2001), Pereira and Stern (1999b, 2000a,b) and Pereira and Wechsler (1993).

Hardy-Weinberg equilibrium
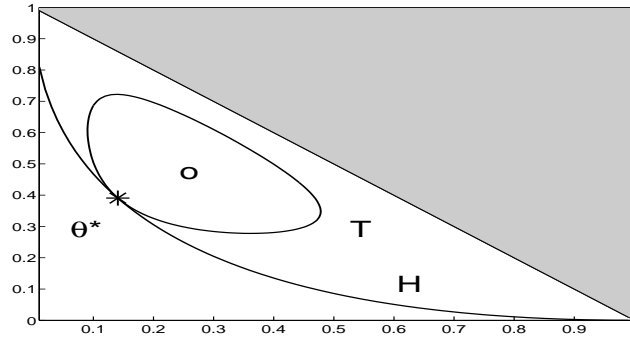
Figure A.2: H-W Hypothesis and Tangential Set

Figure A.2 shows the null set H, the tangential HRSS $\overline{T}$, and the points of constrained and unconstrained maxima, θ^* and $\widehat{\theta}$, for testing Hardy-Weinberg equilibrium law in a population genetics problem, as discussed in Pereira and Stern (1999). In this biological application n is the sample size, x_1 and x_3 are the two homozygote sample counts and $x_2 = n - x_1 - x_3$ is heterozygote sample count. $\theta = [\theta_1, \theta_2, \theta_3]$ is the parameter vector. The posterior and maximum entropy reference densities for this trinomial model, the parameter space and the null set are:

$$p_n(\theta \mid x) \propto \theta_1^{x_1+y_1-1} \theta_2^{x_2+y_2-1} \theta_3^{x_3+y_3-1} \ , \quad r(\theta) \propto \theta_1^{y_1-1} \theta_2^{y_2-1} \theta_3^{y_3-1} \ , \quad y = [0,0,0] \ ,$$

$$\Theta = \{\theta \geq 0 \mid \theta_1 + \theta_2 + \theta_3 = 1\} \ , \quad H = \{\theta \in \Theta \mid \theta_3 = (1 - \sqrt{\theta_1} \ )^2\} \ .$$

Nuisance Parameters

Let us consider the situation where the hypothesis constraint, $H : \ h(\theta) = h(\delta) = 0 \ , \theta = [\delta, \lambda]$ is not a function of some of the parameters, λ. This situation is described by D.Basu in Ghosh (1988):

> *"If the inference problem at hand relates only to δ, and if information gained on λ is of no direct relevance to the problem, then we classify λ as the Nuisance Parameter. The big question in statistics is: How can we eliminate the nuisance parameter from the argument?"*

Basu goes on listing at least 10 categories of procedures to achieve this goal, like using max_λ or $\int d\lambda$, the maximization or integration operators, in order to obtain a projected profile or marginal posterior function, $f(\delta \,|\, x)$. The FBST does not follow the nuisance parameters elimination paradigm, working in the original parameter space, in its full dimension.

A.3   Reference, Invariance and Consistency

In the FBST the role of the reference density, $r(\theta)$ is to make $\overline{ev}(H)$ explicitly invariant under suitable transformations of the coordinate system. Invariance, as used in statistics, is a metric concept. The reference density can be interpreted as a compact and interpretable representation for the reference metric in the original parameter space. This metric is given by information geometry, see section E.5. The natural choice of reference density is an uninformative prior, interpreted as a representation of no information in the parameter space, or the limit prior for no observations, or the neutral ground state for the Bayesian operation.

Standard (possibly improper) uninformative priors include the uniform and maximum entropy densities, see Dugdale (1996) and Kapur (1989) for a detailed discussion. In the H-W example, using the notation above, the uniform density can be represented by $y = [1, 1, 1]$ observation counts, and the standard maximum entropy density can be represented by $y = [0, 0, 0]$ observation counts.

Let us consider the cumulative distribution of the evidence value against the hypothesis, $\overline{V}(c) = \Pr(\overline{ev} \leq c)$, given θ^0, the true value of the parameter. Under appropriate regularity conditions, for increasing sample size, $n \to \infty$, we can say the following:

- If H is false, $\theta^0 \notin H$, then $\overline{ev}$ converges (in probability) to 1, that is, $\overline{V}(0 \leq c < 1) \to 0$.

- If H is true, $\theta^0 \in H$, then $\overline{V}(c)$, the confidence level, is approximated by the function

$$QQ(t, h, c) = Q\left(t - h, Q^{-1}(t, c)\right) , \quad \text{where}$$

$$Q(k, x) = \frac{\Gamma(k/2, x/2)}{\Gamma(k/2, \infty)} , \quad \Gamma(k, x) = \int_0^x y^{k-1} e^{-y} dy ,$$

$t = \dim(\Theta)$, $h = \dim(H)$ and $Q(k, x)$ is the cumulative chi-square distribution with k degrees of freedom. Figure A.3 portrays $QQ(t, h, c) \, Q(t - h, Q^{-1}(t, c))$ for $t = 2 \ldots 4$ and $h = 0 \ldots t - 1$.

Under the same regularity conditions, an appropriate choice of threshold or critical level, $c(n)$, provides a consistent test, τ_c , that rejects the hypothesis if $\overline{\text{ev}}(H) > c$. The empirical power analysis developed in Stern and Zacks (2002) and Lauretto et al. (2003), provides critical levels that are consistent and also effective for small samples.
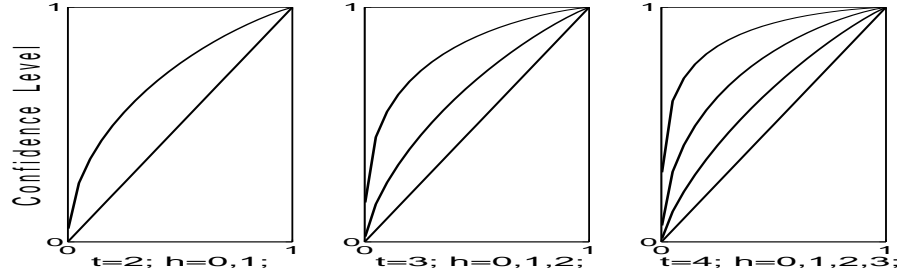
Figure A.3: Test τ_c critical level vs. confidence level

Proof of invariance:

Consider a proper (bijective, integrable, and almost surely continuously differentiable) reparameterization $\omega = \phi(\theta)$. Under the reparameterization, the Jacobian, surprise, posterior and reference functions are:

$$J(\omega) = \left[\frac{\partial\, \theta}{\partial\, \omega} \right] = \left[\frac{\partial\, \phi^{-1}(\omega)}{\partial\, \omega} \right] = \begin{bmatrix} \frac{\partial\, \theta_1}{\partial\, \omega_1} & \cdots & \frac{\partial\, \theta_1}{\partial\, \omega_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial\, \theta_n}{\partial\, \omega_1} & \cdots & \frac{\partial\, \theta_n}{\partial\, \omega_n} \end{bmatrix}$$

$$\widetilde{s}(\omega) = \frac{\widetilde{p}_n(\omega)}{\widetilde{r}(\omega)} = \frac{p_n(\phi^{-1}(\omega))\,|J(\omega)|}{r(\phi^{-1}(\omega))\,|J(\omega)|}$$

Let $\Omega_H = \phi(\Theta_H)$. It follows that

$$\widetilde{s}^* = \sup_{\omega \in \Omega_H} \widetilde{s}(\omega) = \sup_{\theta \in \Theta_H} s(\theta) = s^*$$

hence, the tangential set, $\overline{T} \mapsto \phi(\overline{T}) = \widetilde{\overline{T}}$, and

$$\widetilde{\text{ev}}(H) = \int_{\widetilde{\overline{T}}} \widetilde{p}_n(\omega) d\omega = \int_{\overline{T}} p_n(\theta) d\theta = \overline{\text{ev}}(H).$$

Proof of consistency:

Let $\overline{V}(c) = \Pr(\overline{\text{ev}} \le c)$ be the cumulative distribution of the evidence value against the hypothesis, given θ. We stated that, under appropriate regularity conditions, for

increasing sample size, $n \to \infty$, if H is true, i.e. $\theta \in H$, then $\overline{V}(c)$, is approximated by the function

$$QQ\left(t - h, \mathrm{Q}^{-1}(t, c)\right) \ .$$

Let θ^0, $\widehat{\theta}$ and θ^* be the true value, the unconstrained MAP (Maximum A Posteriori), and constrained (to H) MAP estimators of the parameter θ.

Since the FBST is invariant, we can chose a coordinate system where, the (likelihood function) Fisher information matrix at the true parameter value is the identity, i.e., $J(\theta^0) = I$. From the posterior Normal approximation theorem, see Section 5 of Appendix E, we know that the standarized total difference between $\widehat{\theta}$ and θ^0 converges in distribution to a standard Normal distribution, i.e.

$$\sqrt{n}(\widehat{\theta} - \theta^0) \to N\left(0, J(\theta^0)^{-1}J(\theta^0)J(\theta^0)^{-1}\right) = N\left(0, J(\theta^0)^{-1}\right) = N\left(0, I\right)$$

This standarized total difference can be decomposed into tangent (to the hypothesis manifold) and transversal orthogonal components, i.e.

$$d_t = d_h + d_{t-h} \ , \ dt = \sqrt{n}(\widehat{\theta} - \theta^0) \ , \ d_h = \sqrt{n}(\theta^* - \theta^0) \ , \ d_{t-h} = \sqrt{n}(\widehat{\theta} - \theta^*) \ .$$

Hence, the total, tangent and transversal distances (L^2 norms), $||d_t||$, $||d_h||$ and $||d_{t-h}||$, converge in distribution to chi-square variates with, respectively, t, h and $t - h$ degrees of freedom.

Also from, the MAP consistency, we know that the MAP estimate of the Fisher information matrix, $\widehat{J}$, converges in probability to true value, $J(\theta^0)$.

Now, if X_n converges in distribution to X, and Y_n converges in probability to Y, we know that the pair $[X_n, Y_n]$ converges in distribution to $[X, Y]$. Hence, the pair $[||d_{t-h}||, \widehat{J}]$ converges in distribution to $[x, J(\theta^0)]$, where x is a chi-square variate with $t - h$ degrees of freedom. So, from the continuous mapping theorem, the evidence value against H, $\overline{ev}(H)$, converges in distribution to $\overline{e} = \mathrm{Q}(t, x)$, where x is a chi-square variate with $t - h$ degrees of freedom.

Since the cumulative chi-square distribution is an increasing function, we can invert the last formula, i.e., $\overline{e} = \mathrm{Q}(t, x) \leq c \Leftrightarrow x \leq \mathrm{Q}^{-1}(t, c)$. But, since x in a chi-square variate with $t - h$ degrees of freedom,

$$\Pr(\overline{e} \leq c) = \mathrm{Q}\left(t - h, \mathrm{Q}^{-1}(t, c)\right) \ , \quad \text{Q.E.D.}$$

A similar argument, using a non-central chi-square distribution, proves the other asymptotic statement.

A.4 Loss Functions

In orthodox decision theoretic Bayesian statistics, a significance test is legitimate if and only if it can be characterized as an Acceptance (A) or Rejection (R) decision procedure defined by the minimization of the posterior expectation of a loss function, Λ. Madruga (2001) gives the following family of loss functions characterizing the FBST. This loss function is based on indicator functions of θ being or not in the tangential set $\overline{T}$:

$$\Lambda(R, \theta) = a\, I(\theta \notin \overline{T}) \quad , \quad \Lambda(A, \theta) = b + d\, I(\theta \in \overline{T})$$

The interpretation of this loss function is as follows: If $\theta \in \overline{T}$ we want to reject H, for θ is more probable than anywhere on H; If $\theta \in T$ we want to accept H, for θ is less probable than anywhere on H. The minimization of this loss function gives the optimal test:

$$\text{Accept } H \text{ iff } \text{ev}(H) \geq \varphi = (b + c)/(a + c) \,.$$

Note that this loss function is dependent on the observed sample (via the likelihood function), on the prior, and on the reference density, stressing the important point of non-separability of utility and probability, see Kadane and Winkler (1987) and Rubin (1987).

This type of loss function can be easily adapted in order to provide an asymptotic indicator checking if the true parameter belongs to the hypothesis set, $I(\theta^0 \in H)$. Consider the *tangential reference mass*,

$$\overline{m} = \left[\int_{\overline{T}(s^*)} r(\theta) d\theta \right]^{\gamma}$$

If $\gamma = 1$, $\overline{m}$ is the reference density mass of the tangencial set. If $\gamma = 1/t$, $\overline{m}$ is a pseudo-distance from $\widehat{\theta}$ to θ^*. Consider also a threshold of form $\varphi_1 = b\overline{m}$ or $\varphi_2 = b\overline{m}/(a + \overline{m})$, $a, b > 0$, in the expression of the optimal test above.

If $\theta^0 \notin H$, then $\widehat{\theta} \to \theta^0$ and $\theta^* \to \theta^{0*}$, where $\theta^{0*} \neq \theta^0$, therefore $||\widehat{\theta} - \theta^*|| \to c_1 > 0$. But the standarized posterior, p_n, converges to a normal distribution centered on θ^0. Hence, $\overline{m} \to c_2 > 0$ and $\varphi \to c_3 > 0$. Finally, since $\text{ev}(H) \to 0$, $\Pr(\text{ev}(H) > \varphi) \to 0$.

If $\theta^0 \in H$, then $\widehat{\theta} \to \theta^0$ and $\theta^* \to \theta^0$, therefore $||\widehat{\theta} - \theta^*|| \to 0$. Hence, $\overline{m} \to 0$ and $\varphi \to 0$. But $\text{ev}(H)$ converges to a propper distribution, see section A.3, and, therefore, $\Pr(\text{ev}(H) > \varphi) \to 1$.

A.5 Belief Calculi and Support Structures

Many standard Belief Calculi can be formalized in the context of Abstract Belief Calculus, ABC, see Darwiche and Ginsberg (1992), Darwiche (1993) and Stern (2003). In a

Support Structure, $\langle \Phi, \oplus, \oslash \rangle$, the first element is a Support Function, Φ, on a universe of statements, $\mathcal{U}$. Null and full support values are represented by **0** and **1**. The second element is a support Summation operator, $\oplus$, and the third is a support Scaling or Conditionalization operator, $\oslash$. A Partial Support Structure, $\langle \Phi, \oplus \rangle$, lacks the scaling operation.

The Support Summation operator, $\oplus$, gives the support value of the disjunction of any two logically disjoint statements from their individual support values, i.e.,

$$\neg(A \wedge B) \Rightarrow \Phi(A \vee B) = \Phi(A) \oplus \Phi(B) \ .$$

The Support Scaling operator, $\oslash$, gives the conditional support value of B given A from the unconditional support values of A and the conjunction $C = A \wedge B$, i.e.,

$$\Phi_A(B) = \Phi(A \wedge B) \oslash \Phi(A) \ .$$

Support structures for some standard belief calculi are given in Table A.1, where the support value of two statements their conjunction are given by $a = \Phi(A)$, $b = \Phi(B)$, $c = \Phi(C = A \wedge B)$.

In Table A.1, the relation $a \preceq b$ indicates that the value a represents a stringer support than the value b. Darwiche and Ginsberg (1992) and Darwiche (1993) also give a set o axioms defining the essential functional properties of a (partial) support function. Stern (2003) shows that the support $\Phi(H) = \text{ev}(H)$ complies with all these axioms.

Table A.1: Support structures for some belief calculi, $c = \Phi(C = A \wedge B)$.

$\Phi(\mathcal{U})$	$a \oplus b$	**0**	**1**	$a \preceq b$	$c \oslash a$	Calculus
$\{0,1\}$	$\max(a,b)$	0	1	$a \leq b$	$\min(c,a)$	Classical Logic
$[0,1]$	$a+b$	0	1	$a \leq b$	c/a	Probability
$[0,1]$	$\max(a,b)$	0	1	$a \leq b$	c/a	Possibility
$\{0\ldots\infty\}$	$\min(a,b)$	∞	0	$b \leq a$	$c-a$	Disbelief

In the FBST, the support values, $\Phi(H) = \text{ev}(H)$, are computed using standard probability calculus on Θ which has an intrinsic conditionalization operator. The computed evidences, on the other hand, have a possibilistic summation, i.e., the value of evidence in favor of a composite hypothesis $H = A \vee B$, is the most favorable value of evidence in favor of each of its terms, i.e., $\text{ev}(H) = \max\{\text{ev}(A), \text{ev}(B)\}$. It is impossible however to define a simple scaling operator for this possibilistic support that is compatible with the FBST's evidence, ev, as it is defined.

Hence, two belief calculi are in simultaneous use in the FBST setup: $\text{ev}(H)$ constitutes a possibilistic partial support structure coexisting in harmony with the probabilistic support structure given by the posterior probability measure, $p_n(\theta)$, in the parameter space.

Requirements (V) and (VI), i.e. *no ad hoc artifice* and *possibilistic support*, find a rich interpretation in the juridical or legal context, where they correspond to the some of the most basic juridical principles, see Stern (2003).

Onus Probandi is a basic principle of legal reasoning, also known as Burden of Proof, see Gaskins (1992) and Kokott (1998). It also manifests itself in accounting through the Safe Harbor Liability Rule:

> *"There is no liability as long as there is a reasonable basis for belief, effectively placing the burden of proof (Onus Probandi) on the plaintiff, who, in a lawsuit, must prove false a defendant's misstatement, without making any assumption not explicitly stated by the defendant, or tacitly implied by an existing law or regulatory requirement."*

The Most Favorable Interpretation principle, which, depending on the context, is also known as Benefit of the Doubt, *In Dubito Pro Reo*, or Presumption of Innocence, is a consequence of the Onus Probandi principle, and requires the court to consider the evidence in the light of what is most favorable to the defendant.

> *"Moreover, the party against whom the motion is directed is entitled to have the trial court construe the evidence in support of its claim as truthful, giving it its most favorable interpretation, as well as having the benefit of all reasonable inferences drawn from that evidence."*

A.6 Sensitivity and Inconsistency

For a given prior, likelihood and reference density, let $\eta = \text{ev}(H; p_0, L_x, r)$ denote the e-value supporting H. Let $\eta', \eta'' \ldots$ denote the e-value with respect to references $r', r'' \ldots$. The degree of inconsistency of the e-value supporting H, induced by a set of references, $\{r, r', r'' \ldots\}$ is defined by the index

$$I\{\eta, \eta', \eta'' \ldots\} = \max\{\eta, \eta', \eta'' \ldots\} - \min\{\eta, \eta', \eta'' \ldots\}$$

The same index can be used to study the degree of inconsistency of the e-value induced by a set of priors, $\{p_0, p_0', p_0'' \ldots\}$. One could also study the sensitivity of the e-value to a set of vitual sample sizes, $\{1n, \gamma'n, \gamma''n \ldots\}$, $\gamma \in [0, 1]$, corresponding to scalled likelihoods, $\{L, L^{\gamma'}, L^{\gamma''} \ldots\}$. This intuitive measure of inconsistency can be made rigorous in the context of paraconsistent logic and bilattice structures, see Abe et al. (1998), Alcantara et al. (2002), Arieli and Avron (1996), Costa (1963), Costa and Subrahmanian (1989) and Costa et al. (1991), (1999).

The bilattice $B(C, D) = \langle C \times D, \leq_k, \leq_t \rangle$, given two complete lattices, $\langle C, \leq_c \rangle$, and $\langle D, \leq_d \rangle$, has two orders, the knowledge order, $\leq_k$, and the truth order, $\leq_t$, given by:

$$\langle c_1, d_1 \rangle \leq_k \langle c_2, d_2 \rangle \quad \Leftrightarrow \quad c_1 \leq_c c_2 \text{ and } d_1 \leq_d d_2$$
$$\langle c_1, d_1 \rangle \leq_t \langle c_2, d_2 \rangle \quad \Leftrightarrow \quad c_1 \leq_c c_2 \text{ and } d_2 \leq_d d_1$$

The standard interpretation is that C provides the "credibility" or value in favor of a hypothesis (or statement) H, and D provides the "doubt" or value against H. If $\langle c_1, d_1 \rangle \leq_k \langle c_2, d_2 \rangle$, then we have more information (even if inconsistent) about situation 2 than 1. Analogously, if $\langle c_1, d_1 \rangle \leq_t \langle c_2, d_2 \rangle$, then we have more reason to trust (or believe) situation 2 than 1 (even if with less information).

For each of the bilattice orders we define a join and a meet operator, based on the join and the meet operators of the single lattices orders. More precisely, $\sqcup_k$ and $\sqcap_k$, for the knowledge order, and $\sqcup_t$ and $\sqcap_t$, for the truth order, are defined by the folowing equations:

$$\langle c_1, d_1 \rangle \sqcup_k \langle c_2, d_2 \rangle = \langle c_1 \sqcup_c c_2, d_1 \sqcup_d d_2 \rangle, \langle c_1, d_1 \rangle \sqcap_k \langle c_2, d_2 \rangle = \langle c_1 \sqcap_c c_2, d_1 \sqcap_d d_2 \rangle$$

$$\langle c_1, d_1 \rangle \sqcup_t \langle c_2, d_2 \rangle = \langle c_1 \sqcup_c c_2, d_1 \sqcap_d d_2 \rangle, \langle c_1, d_1 \rangle \sqcap_t \langle c_2, d_2 \rangle = \langle c_1 \sqcap_c c_2, d_1 \sqcup_d d_2 \rangle$$

The "unit square" bilattice, $\langle [0,1] \times [0,1], \leq, \leq \rangle$ has been routinely used to represent fuzzy or rough pertinence relations, logical probabilistic annotations, etc. The lattice $\langle [0,1], \leq \rangle$ is the standard unit interval, where the join and meet coincide with the max and min operators, $\sqcup = \max$ and $\sqcap = \min$.

In the unit square bilattice the "truth", "false", "inconsistency" and "indetermination" extremes are t, f, $\top$, $\bot$, whose coordinates are given in Figure A.4. As a simple example, let region R be the convex hull of the four vertices n, s, e and w, given in Figure A.4. Points kj, km, tj and tm are the knowledge and truth join and meet, over $r \in R$.

In the unit square bilattice, the degree of trust and degree of inconsistency for a point $x = \langle c, d \rangle$ are given by BT $(\langle c, d \rangle) = c - d$, and BI $(\langle c, d \rangle) = c + d - 1$, a convenient linear reparameterization of $[0,1]^2$, to $[-1, +1]^2$. Figure A.4 also compares the credibility-doubt and trust-inconsistency coordinates.

Let $\eta = \text{ev}(H)$, and $\overline{\eta} = \overline{\text{ev}}(H) = 1 - \text{ev}(H)$. The point $x = \langle \eta, \overline{\eta} \rangle$ in the unit square bilattice, represents herein a single evidence. Since BI$(x) = 0$, such a point is consistent. It is also easy to verify that for the multiple e-values, the definition of degree of inconsistency given above, is the degree of inconsistency of the knowledge join of all the single evidence points, i.e.,

$$I(\eta, \eta', \eta'' \dots) = \text{BI}\left(\langle \eta, \overline{\eta} \rangle \sqcup_k \langle \eta', \overline{\eta}' \rangle \sqcup_k \langle \eta'', \overline{\eta}'' \rangle \dots \right) .$$

Negation type operators are not an integral part of the bilattice structure but, in the unit square, one can define negation as $\neg \langle c, d \rangle = \langle d, c \rangle$, and conflation as $- \langle c, d \rangle =$
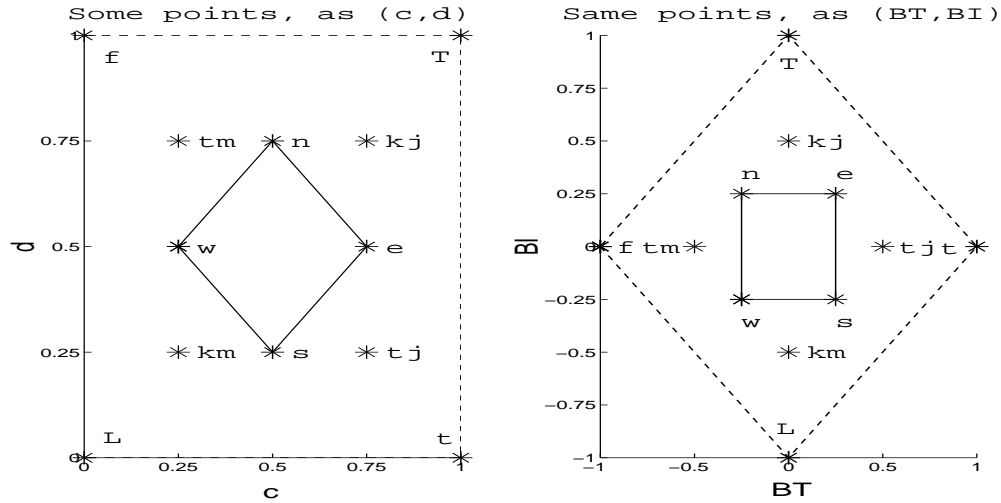
Figure A.4: credibility-doubt and trust-inconsistency coordinates

$\langle 1 - c, 1 - d \rangle$, so that negation reverses trust, but preserves knowledge, and conflation reverses knowledge, but preserves trust.

As an example of sensitivity analysis we use the HW model with the standard uninformative references, the uniform and the maximum entropy densities, represented by $[1, 1, 1]$ and $[0, 0, 0]$ observation counts. For a motivation for this particular analysis, see the observations at the end of section E.5. Between these two uninformative references, we also consider perturbation references corresponding to $[0, 1, 1]$, $[1, 0, 1]$ and $[1, 1, 0]$ observation counts. Each of these references can be interpreted as the exclusion of a single observation of the corresponding type from the observed data set.
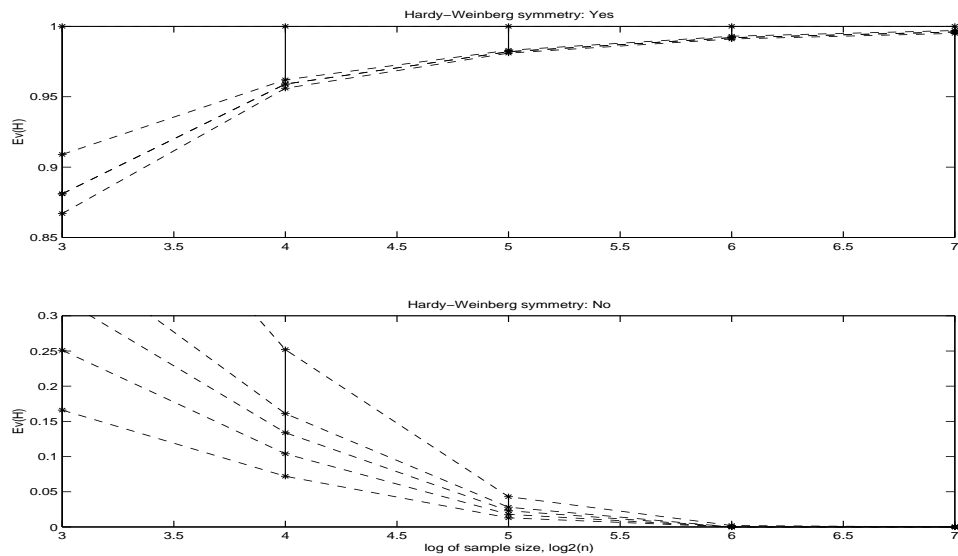
Figure A.5: Sensitivity analysis

The *e*-values in the example are calculated using two sample proportions, $[x_1, x_2, x_3]$ $= n[1/4, 1/4, 1/2]$ and $= n[1/4, 1/2, 1/4]$. The first exhibits the HW hypothesis symmetry, the second does not. The log 2 of sample size, $\log_2(n)$, ranged from 3 to 7. In Figure A.5, the *e*-values corresponding to each choice of reference, are given by an interpolated dashed line. The interpretation of the vertical interval (solid bars) between the dashed lines is similar to that of the usual statistical error bars. However, the uncertainty represented by these bars does not have a probabilistic nature, being rather a possibilistic measure of inconsistency, defined in the partial support structure given by the FBST evidence value, see Stern (2004).

A.7   Complex Models and Compositionality

The relationship between the credibility of a complex hypothesis, H, and those of its constituent elementary hypothesis, $H^{(i,j)}$, in the independent setup, can be analyzed under the FBST, see Borges and Stern (2006) for precise definitions, and detailed interpretation.

Let us consider elementary hypotheses, $H^{(i,j)}$, in k independent constituent models, M^j, and the complex or composit hypothesis H, equivalent to a (homogeneous) logical composition (disjunction of conjunctions) of elementary hypotheses, in the composit product model, M.

The possibilistic nature of the *e*-value measure makes it easy to compute the support for disjunctive complex hypotheses. Conjunction of elementary hypotheses require a more sophisticated analysis. First we must observe that knowing the *e*-values of the elementary hypotheses is not enough to know the *e*-value of the conjunction; Elementary *e*-values can give only lower and upper bounds to the support for the conjunction. Figure A.6 illustrates these bounds, and also the following results, for further details see Borges and Stern (2006). For conjunctive compositions, the models' truth functions, W^j, are the key element for the required algebraic manipulation, as stated in the next result.

If H is expressed in HDNF or Homogeneous Disjunctive Normal Form,

$$H \;=\; \bigvee_{i=1}^{q} \bigwedge_{j=1}^{k} H^{(i,j)} \;,\quad M^{(i,j)} = \{\Theta^j, H^{(i,j)}, p_0^j, p_n^j, r^j\} \;,$$

$$M = \{\Theta, H, p_0, p_n, r\} \;,\quad \Theta = \prod_{j=1}^{k} \Theta^j \;,\quad p_n = \prod_{j=1}^{k} p_n^j \;,\quad r = \prod_{j=1}^{k} r^j \;;$$

then the e-value supporting H is

$$\mathrm{ev}(H) = \; \mathrm{ev}\left(\bigvee_{i=1}^{q} \bigwedge_{j=1}^{k} H^{(i,j)}\right) = \; W\left(\max_{i=1}^{q} \prod_{j=1}^{k} s^{*(i,j)}\right) =$$

$$W\left(\max_{i=1}^{q} s^{*i}\right) = \; \max_{i=1}^{q} W\left(s^{*i}\right) = \; \max_{i=1}^{q} \mathrm{ev}\left(\bigwedge_{j=1}^{k} H^{(i,j)}\right) = \; \max_{i=1}^{q} \mathrm{ev}\left(H^i\right) \;;$$

where the cumulative surprise distribution of the composite model, $W(v)$, is given by the Mellin convolution operation, see Springer (1979), defined as

$$W = \bigotimes_{1 \leq j \leq k} W^j \ , \quad W^1 \otimes W^2(v) \ = \ \int_0^\infty W^1(v/y) W^2(dy) \ .$$

The probability distribution of the product of two independent positive random variables is the Mellin convolution of each of their distributions. From this interpretation, the we immediately see that $\otimes$ is a commutative and associative operator.

Mirroring Wittgenstein, in the FBST context, we can call the e-value, $\mathrm{ev}(H)$, the cumulative surprise distribution, $W(v)$, and the Mellin convolution operation, $\otimes$, respectively, truth value, truth function, and truth operation.

Finally, we observe that, in the extreme case of null-or-full support, that is, when, for $1 \leq i \leq q$ and $1 \leq j \leq k$, $s^{*(i,j)} = 0$ or $s^{*(i,j)} = \widehat{s}^j$, the evidence values (or, in this context, truth values) of the constituent elementary hypotheses are either 0 or 1, and the conjunction and disjunction composition rules of classical logic hold.

Numerical Aspects

In appendix G we detail an efficient Monte Carlo algorithm for computing $\mathrm{ev}(H; p_n, r)$. In this algorithm, the bulk of the work consists in generating random points in the parameter space, $\theta^j \in \Theta$, and evaluating the surprise function, $s^j = s(\theta^j)$. The Monte Carlo algorithm proceeds updating several accumulators based on the tangential set "hit indicator",

$$I^*(\theta^j; p_n, r) = \mathbf{1}(\theta^j \in \overline{T}) = \mathbf{1}(s(\theta^j) > s^*) \ .$$

In order to compute a k-step function approximation of $W(v)$, we only have to split the surprise range interval, $[0, \widehat{s}]$ with a vector of k intermediate points, $0 < s^1 < s^2 < \ldots s^h < s^* < s^{h+1} < \ldots s^k < \widehat{s}$, and set up a set of vector accumulators based on the vector threshold indicator, $I^k(\theta^j; p_n, r) = \mathbf{1}(s(\theta^j) > s^k)$. Updating the vector accumulators usualy imposes only a small overhead on the Monte Carlo algorithm.

Numerical convolutions of step functions can be easily computed with the help of good condensation procedures, see Kaplan and Lin (1987). For alternative approaches to numerical convolution see Springer (1979) and Williamson (1989). In the case of dependent models, the composite truth function can be solved with the help of analytical and numerical copulas, see Cherubini et al. (2004), Mari and Kotz (2001) and Nelsen (2006).
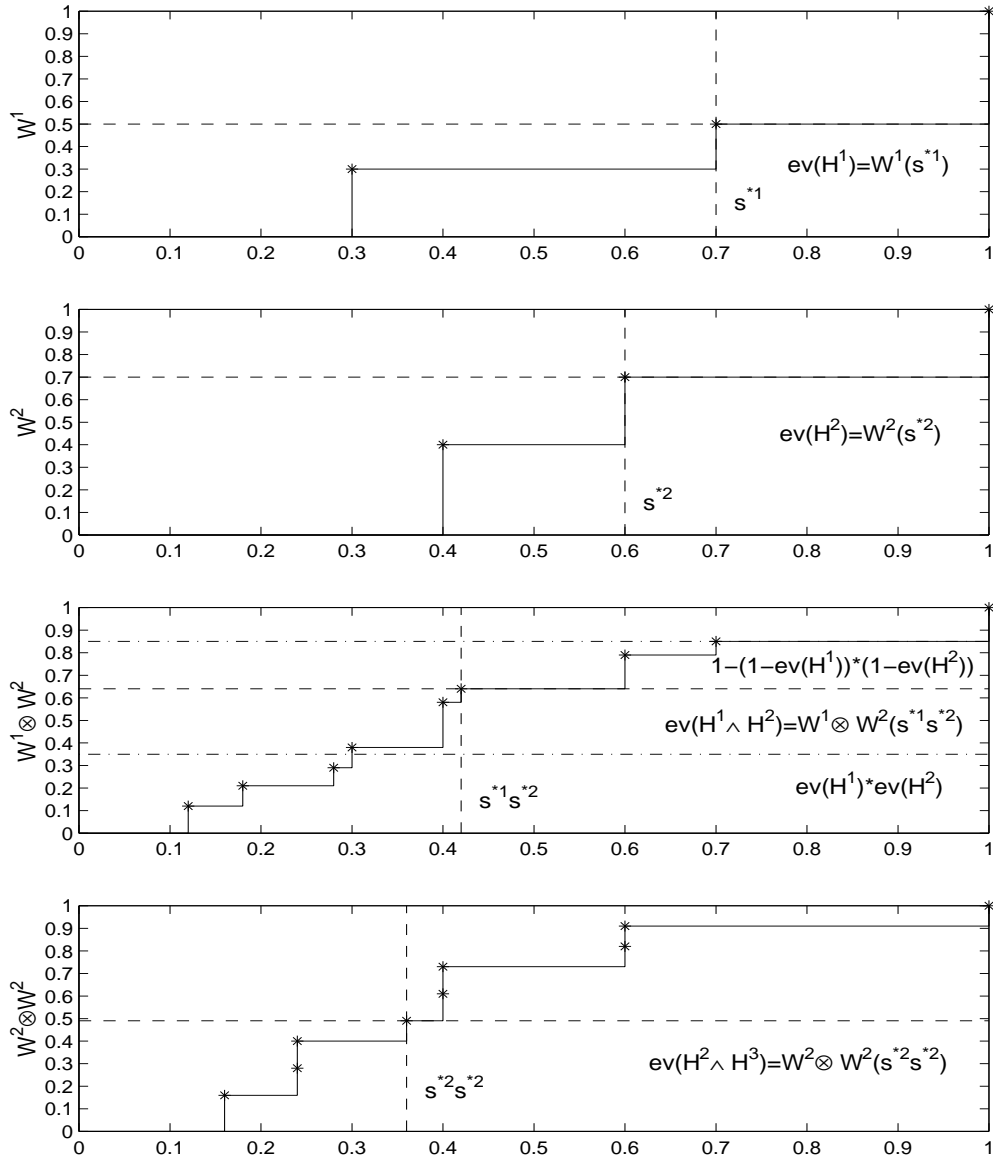
Fig A.6. Subplots 1,2: W^j, s^{*j}, and $\mathrm{ev}(H^j)$, for $j = 1, 2$;
Subplot 3: $W^1 \otimes W^2$, $s^{*1}s^{*2}$, $\mathrm{ev}(H^1 \wedge H^2)$ and bounds;
Subplot 4: Structure M^3 is an independent replica of M^2,
$\mathrm{ev}(H^1) < \mathrm{ev}(H^2)$, but $\mathrm{ev}(H^1 \wedge H^3) > \mathrm{ev}(H^2 \wedge H^3)$.

Appendix B

Binomial, Dirichlet, Poisson and Related Distributions

This essay has been published as Pereira and Stern (2008).

The matrix notation used in this section is defined in section F.1.

B.1   Introduction and Notation

This essay presents important properties of the distributions used for categorical data analysis. Regardless of the population size being known or unknown, or the specific observational stopping rule, the Bernoulli Processes generates the sampling distributions considered. On the other hand, the Gamma distribution generates the prior and posterior distributions obtained: Gamma, Gamma-Poisson, Dirichlet, and Dirichlet-Multinomial. The Poisson Processes as generator of sampling distributions is also considered.

The generation form of the discrete sampling distributions presented in Section 2 is, in fact, a characterization method of such distributions. If one recalls that all the distribution classes being mixed are complete classes and are Blackwell sufficient for the Bernoulli processes, the mixing distributions are unique. This characterization method is completely described in Basu and Pereira (1983).

Section 9 describes the Reny-Aczel characterization of the Poisson distribution. Although it could be thought as a de Finetti type characterization this characterization is based on alternative requirements. While de Finetti chaparcterization is based on a permutable infinite 0-1 process, Reny-Aczek characterization is based on a homogeneous Markov process in a finite interval, generating finite discrete Markov Chains. Using Reny-Aczel characterization, together with Theorem 4, one can obtain a characterization of Multinomial distributions.

Section 7 describes the Dirichlet of Second Kind. In this section we also show how to use a multivariate normal approximation to the logarithm of a random vector distributed as Dirichlet of Second Kind, and a log-normal approximation to a Gamma distribution, see Aitchison and Shen (1980). In many examples of the authors' consulting practice these approximations proved to be a powerful modeling tool, leading to efficient computational procedures.

The development of the theory in this essay is self contained, seeking a unified treatment of a large variety of problems, including finite and infinite populations, contingency tables of arbitrary dimension, deficiently categorized data, logistic regressions, etc. These models also present a way of introducing non parametric solutions.

The singular representation adopted is unusual in statistical texts. This singular representation makes it simpler to extend and generalize the results and greatly facilitates numerical and computational implementation. In this essay, corollaries, lemmas, propositions and theorems are numbered sequentially.

We introduce the following notation for observation matrices, and respective summation vectors:

$$U = [u^1, u^2, \ldots] \ , \ U^{1:n} = [u^1, u^2, \ldots u^n] \ , \ x^n = U^{1:n}\mathbf{1} = \sum\nolimits_{j=1}^{n} u^j \ .$$

The tilde accent indicates some form of normalization like, for example, $\widetilde{x} = (1/\mathbf{1}'x)x$.

Lemma 1: If $u^1, \ldots u^n$ are i.i.d random vectors,

$$x = U^{1:n}\mathbf{1} \Rightarrow \mathrm{E}(x) = n\,\mathrm{E}(u^1) \text{ and } \mathrm{Cov}(x) = n\mathrm{Cov}(u^1) \ .$$

The first result is trivial. For the second result, we only have to remember the transformation properties of for the expectation and covariance operators by a linear operation on their argument,

$$E(AY + b) = AE(Y) + b \ , \ \ \mathrm{Cov}(AY + b) = A\mathrm{Cov}(Y)A' \ ,$$

and write

$$\begin{aligned}
\mathrm{Cov}(x) &= \mathrm{Cov}(U^{1:n}\mathbf{1}) \\
&= \ \mathrm{Cov}\left((\mathbf{1}' \otimes I)\,\mathrm{Vec}(U^{1:n})\right) \ = \ (\mathbf{1}' \otimes I)\left(I \otimes \mathrm{Cov}(u^1)\right)(\mathbf{1} \otimes I) \\
&= \ \left(\mathbf{1}' \otimes \mathrm{Cov}(u^1)\right)(\mathbf{1} \otimes I) \ = \ n\mathrm{Cov}(u^1) \ .
\end{aligned}$$

B.2   The Bernoulli Process

Let us consider a sequence of random vectors $u^1, u^2, \ldots$ where, $\forall u^i$ can assume only two values

$$I^1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \text{ or } I^2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \text{ where } I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

representing success or failure. That is, u^i can assume the value of any column of the identity matrix, I. We say that u^i is of class k, $c(u^i) = k$, iff $u^i = I^k$, $k \in [1, 2]$.

Also assume that (in your opinion), this sequence is exchangeable, that is, if $p = [p(1), p(2), \ldots p(n)]$ is a permutation of $[1, 2, \ldots n]$, than, $\forall n, p$,

$$\Pr\left(u^1, \ldots u^n\right) = \Pr\left(u^{p(1)}, \ldots u^{p(n)}\right) .$$

Just from this exchangeability constraint, that can be interpreted as saying that the index labels are non informative, de Finetti Theorem establishes the existence of an unknown vector

$$\theta \in \Theta = \{\mathbf{0} \leq \theta = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix} \leq \mathbf{1} \mid \mathbf{1}'\theta = 1\}$$

such that, conditionally on θ, $u^1, u^2, \ldots$ are mutually independent, and the conditional probability of $\Pr(u^i = I^k \mid \theta)$ is θ_k, i.e.

$$(u^1 \amalg u^2 \amalg \ldots) \mid \theta \text{ or } \coprod_{i=1}^{\infty} u_i \mid \theta , \text{ and } \Pr(u^i = I^k \mid \theta) = \theta_k .$$

Vector θ is characterized as the limit of proportions

$$\theta = \lim_{n \to \infty} \frac{1}{n} x^n , \quad x^n = U^{1:n}\mathbf{1} = \sum_{j=1}^{n} u^j .$$

Conditionally on θ, the sequence $u^1, u^2, \ldots$ receives the name of Bernoulli process. As we shall see, many well known discrete distributions can be obtained from transformations of this process.

The expectation and covariance (conditionally on θ) of any vector in the sequence are:

- $\mathrm{E}(u^i) = \theta$,

- $\mathrm{Cov}(u^i) = \mathrm{E}\left(u^i \otimes (u^i)'\right) - \mathrm{E}\left(u^i\right) \otimes \mathrm{E}\left((u^i)'\right) = \mathrm{diag}(\theta) - \theta \otimes \theta'$.

When the summation domain $1 : n$, is understood, we may use the relaxed notation x instead of x^n. We also define the Delta operator, or "pointwise power product" between two vectors of same dimension: Given θ, and x, $n \times 1$,

$$\theta \triangle x \equiv \prod_{i=1}^{n}(\theta_i)^{x_i} .$$

A stopping rule, δ, establishes, for every $n = 1, 2, \ldots$, a decision of observing (or not) u^{n+1}, after the observations $u^1, \ldots u^n$.

For a good understanding of this text, it is necessary to have a clear interpretation of conditional expressions like $x^n \mid n$ or $x_2^n \mid x_1^n$. In both cases we are referring to a unknown

vector, x^n, but with a different partial information. In the first case, we know n, and therefore we know the sum of components, $x_1^n + x_2^n = n$; however, we know neither component x_1^n nor x_2^n. In the second case we only know the first component, of x^n, x_1^n, and do not know the second component, x_2^n, obviously we also do not know the sum, $n = x_1^n + x_2^n$. Just pay attention: We list what we know to the right of the bar and, (unless we have some additional information) everything that can not be deduced from this list is unknown.

The first distribution we are going to discuss is the Binomial. Let $\delta(n)$ be the stopping rule where n is the pre-established number of observations. The (conditional) probability of the observation sequence $U^{1:n}$ is

$$\Pr(U^{1:n} \mid \theta) = \theta \bigtriangleup x^n \ .$$

The summation vector, x^n, has Binomial distribution with parameters n and θ, and we write $x^n \mid [n, \theta] \sim \mathrm{Bi}(n, \theta)$. When n (or $\delta(n)$) is implicit in the context we may write $x \mid \theta$ instead of $x^n \mid [n, \theta]$. The Binomial distribution has the following expression:

$$\Pr(x^n \mid n, \theta) = \left(\begin{array}{c} n \\ x^n \end{array} \right) (\theta \bigtriangleup x^n)$$

where

$$\left(\begin{array}{c} n \\ x \end{array} \right) \equiv \frac{\Gamma(n+1)}{\Gamma(x_1 + 1)\,\Gamma(x_2 + 1)} = \frac{n!}{x_1!\,x_2!} \ \text{and } n = \mathbf{1}'x \ .$$

A good exercise for the reader is to check that expectation vector and the covariance matrix of $x^n \mid [n, \theta]$ have the following expressions:

$$\mathrm{E}(x^n) = n\theta \ \text{ and } \ \mathrm{Cov}(x^n) = n\,(\theta \bigtriangleup \mathbf{1}) \left[\begin{array}{cc} 1 & -1 \\ -1 & 1 \end{array} \right] \ .$$

The second distribution we discuss is the Negative Binomial. Let $\delta(x_1^n)$ be the rule establishing to stop at observation u^n when obtaining a pre-established number of x_1^n successes. The random variable x_2^n, the number of failures he have when we obtain the required x_1^n successes, is called a Negative Binomial with parameters x_1^n and θ. It is not hard to prove that the Negative Binomial distribution $x_2^n \mid [x_1^n, \theta] \sim \mathrm{NB}(x_1^n, \theta)$, has expression, $\forall\, x_2^n \in \mathbb{N}$,

$$\Pr(x^n \mid x_1^n, \theta) \ = \ \frac{x_1^n}{n} \left(\begin{array}{c} n \\ x^n \end{array} \right) (\theta \bigtriangleup x^n) \ = \ \theta_1 \Pr\left((x^n - I^1) \mid (n-1), \theta) \right) \ .$$

Note that, from the definition this distribution, x_1^n is a positive integer number. Nevertheless, we can extend the definition above for any real positive value a, and still obtain a probability function. For this, we use

$$\sum_{j=0}^{\infty} \frac{\Gamma(a+j)}{\Gamma(a)j!} (1-\pi)^j = \pi^{-a} \ , \ \forall\, a \in [0, \infty[\ \text{and } \pi \in]0, 1[\ .$$

The reader is asked to check the last equation, as well as the following expressions for the expectation and variance of x_2^n:

$$\mathrm{E}\left(x_2^n \,|\, x_1^n, \theta\right) = \frac{x_1^n \theta_2}{\theta_1} \quad \text{and} \quad \mathrm{Var}\left(x_2^n \,|\, x_1^n, \theta\right) = \frac{x_1^n \theta_2}{(\theta_1)^2} \ .$$

In the special case of $\delta(x_1^n = 1)$, the Negative Binomial distribution is also known as the Geometric distribution with parameter θ. If a random variables are independent and identically distributed (i.i.d.) as a geometric distribution with parameter θ, then the sum of these variables has Negative Binomial distribution with parameters a and θ.

The third distribution studied in this essay is the Hypergeometric. Going back to the original sequence, $u^1, u^2, ...$, assume that a first observer knows the first N observations, while a second observer knows only a subsequence of $n < N$ of these observations. Since the original sequence, $u^1, u^2, \ldots$, is exchangeable, we can assume, without loss of generality, that the subsequence known to the second observer is the subsequence of the first n observations, $u^1, \ldots u^n$. Using de Finetti theorem, we have that x^n and $x^N - x^n = U^{n+1:N}\mathbf{1}$ are conditionally independent, given θ. That is, $x^n \ \mathrm{II} \ (x^N - x^n)\,|\,\theta$. Moreover, we can write

$$x^n \,|\, [n, \theta] \sim \mathrm{Bi}(n, \theta) \ , \quad x^N \,|\, [N, \theta] \sim \mathrm{Bi}(N, \theta) \ , \quad \text{and}$$

$$(x^N - x^n) \,|\, [(N - n), \theta] \sim \mathrm{Bi}(N - n, \theta) \ .$$

Our goal is to find the distribution function of $x^n \,|\, x^N$. Note that x^N is sufficient for $U^{1:N}$ given θ, and x^n is sufficient for $U^{1:n}$. Moreover $x^n \,|\, [n, x^N]$ has the same distribution of $x^n \,|\, [n, x^N, \theta]$. Using the basic rules of probability calculus and the properties above, we have that

$$
\begin{aligned}
&\Pr(x^n \,|\, n, x^N, \theta) \\
&= \frac{\Pr(x^n, x^N \,|\, n, N, \theta)}{\Pr(x^N \,|\, n, N, \theta)} = \frac{\Pr(x^n, (x^N - x^n) \,|\, n, N, \theta)}{\Pr(x^N \,|\, n, N, \theta)} \\
&= \frac{\Pr(x^n \,|\, n, N, \theta)\,\Pr(x^N - x^n \,|\, n, N, \theta)}{\Pr(x^N \,|\, n, N, \theta)} \ .
\end{aligned}
$$

Hence, $x^n \,|\, [n, x^N]$ has distribution function

$$\Pr(x^n \,|\, n, x^N) = \frac{\dbinom{n}{x^n} \dbinom{N-n}{x^N - x^n}}{\dbinom{N}{x^N}}$$

where $\mathbf{0} \le x^n \le x^N \le N\mathbf{1}$, $\mathbf{1}'x^n = n$, $\mathbf{1}'x^N = N$.

This is the vector representation of the Hypergeometric probability distribution.

$$x^n \,|\, [n, x^N] \sim \mathrm{Hy}(n, N, x^N) \ .$$

The reader is asked to check the following expressions for the expectation and (conditional) covariance of $x^n \,|\, [n, N, x^N]$, and covariance of u^i and u^j, $i, j \leq n$:

$$\mathrm{E}(x^n) = \frac{n}{N}\, x^N \quad \text{and} \quad \mathrm{Cov}(x^n) = \frac{n(N-n)}{(N-1)}\, (x^N \triangle \mathbf{1}) \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

$$\mathrm{Cov}(u^i, u^j \,|\, x^N) = \frac{1}{(N-1)N^2}\, (x^N \triangle \mathbf{1}) \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \ .$$

We finish this section presenting the derivation of the Beta-Binomial distribution. Let us assume that the first observer observed x_2^n failures, until observing a pre-established number of x_1^n successes. A second observer makes more observations, observing x_2^N failures until completing the pre-established number of x_1^N successes, $x_1^n < x_1^N$.

Since x_1^n and x_1^N are pre-established, we can write

$$x_2^N \,|\, \theta \sim \mathrm{NB}(x_1^N, \theta) \ , \quad x_2^n \,|\, \theta \sim \mathrm{NB}(x_1^n, \theta)$$

$$(x_2^N - x_2^n) \,|\, \theta \sim \mathrm{NB}(x_1^N - x_1^n, \theta) \quad \text{and} \quad x_2^n \ \mathrm{II} \ (x_2^N - x_2^n) \,|\, \theta \ .$$

As before, our goal is to describe the distribution of $x_2^n \,|\, [x_1^n, x^N]$. If one notices that $[x_1^n, x^N]$ is sufficient for $[x^n, (x^N - x^n)]$, with respect to θ, the problem becomes similar to the Hypergeometric case, and one can obtain

$$\Pr(x_2^n \,|\, x_1^n, x^N) = \frac{x_2^N!\,\Gamma(x_1^N)}{\Gamma(x_2^N + x_1^N)}\, \frac{\Gamma(x_2^n + x_1^n)}{x_2^n!\,\Gamma(x_1^n)}\, \frac{\Gamma(x_2^N - x_2^n + x_1^N - x_1^n)}{(x_2^N - x_2^n)!\,\Gamma(x_1^N - x_1^n)} \ ,$$

$$x_2^n \in \{0, 1, ..., x_2^N\} \ .$$

This is the distribution function of a random variable called Beta Binomial with parameters x_1^n and x^N.

$$x_2^n \,|\, (x_1^n, x^N) \sim \mathrm{BB}(x_1^n, x^N) \ .$$

The properties of this distribution will be studied in the general case of the Dirichlet-Multinomial, in the following sections.

Generalized categories for $k > 2$ can be represented by the orthonormal base $I^1, I^2, \ldots I^k$, i.e., the columns of the k-dimensional identity matrix. The Multinomial and Hypergeometric multivariate distributions, presented in the next sections, are distributions derived of this basic generalization.

B.3   Multinomial Distribution

Let u^i, $i = 1, 2, \ldots$ be random vectors with possible results in the set of columns of the m-dimensional identity matrix, $I^k, k \in 1:m$. We say that u^i is of class k, $c(u^i) = k$, iff $u^i = I^k$.

Let $\theta \in [0, 1]^m$ be the vector of probabilities for an observation of class k in a m-variate Bernoulli process, i.e.,

$$\Pr(u^i = I^k \,|\, \theta) = \theta_k \;,\; \mathbf{0} \leq \theta \leq \mathbf{1} \;,\; \mathbf{1}'\theta = 1 \;.$$

Like in the last section, let U

$$U = [u^1, u^2, \ldots] \text{ and } x^n = U^{1:n}\mathbf{1} \;.$$

Definition: If the knowledge of θ makes the vectors u^i independent, then the (conditional) distribution of x^n given θ is the Multinomial distribution of order m with parameters n and θ, given by

$$\Pr(x^n \,|\, n, \theta) = \left(\begin{array}{c} n \\ x^n \end{array} \right) (\theta \,\triangle\, x^n)$$

where

$$\left(\begin{array}{c} n \\ x \end{array} \right) \equiv \frac{\Gamma(n+1)}{\Gamma(x_1+1)\ldots\Gamma(x_m+1)} = \frac{n!}{x_1!\ldots x_m!} \text{ and } n = \mathbf{1}'x \;.$$

We represent the m-Multinomial distribution writing

$$x^n \,|\, [n, \theta] \sim \mathrm{Mn}_m(n, \theta) \;.$$

When $m = 2$, we have the binomial case.

Let us now examine some properties of the Multinomial distribution.

Lemma 2: If $x \,|\, \theta \sim \mathrm{Mn}_m(n, \theta)$ then the (conditional) expectation and covariance of x are

$$\mathrm{E}(x) = n\theta \text{ and } \mathrm{Cov}(x) = n(\mathrm{diag}(\theta) - \theta \otimes \theta') \;.$$

Proof: Analogous to the binomial case.

The next result presents a characterization of the Multinomial in terms of the Poisson distribution.

Lemma 3: Reproductive property of the Poisson distribution.

$$x_i \sim \mathrm{Ps}(\lambda_i) \;\Rightarrow\; \mathbf{1}'x \,|\, \lambda \sim \mathrm{Ps}(\mathbf{1}'\lambda) \;.$$

that is, the sum of (independent) Poisson variates is also Poisson.

Theorem 4: Characterization of the Multinomial by the Poisson.

Let $x = [x_1, ..., x_m]'$ be a vector with independent Poisson distributed components with parameters in the known vector $\lambda = [\lambda_1, ..., \lambda_m]' > 0$. Let n be a positive integer. Then, given λ,

$$x \,|\, [n = \mathbf{1}'x, \lambda] \quad \sim \mathrm{Mn}_m(n, \theta) \text{ where } \theta = \frac{1}{\mathbf{1}'\lambda}\lambda \ .$$

Proof: The joint distribution of x, given λ is

$$\Pr(x \,|\, \lambda) = \prod_{k=1}^{m} \frac{e^{-\lambda_k}\lambda_i^{x_k}}{x_k!} \ .$$

Using the Poisson reproductive property,

$$
\begin{aligned}
&\Pr\left(x \,|\, \mathbf{1}'x = n, \lambda\right) \\
&= \frac{\Pr\left(\mathbf{1}'x = n \wedge x \,|\, \lambda\right)}{\Pr\left(\mathbf{1}'x = n \,|\, \lambda\right)} \quad = \quad \delta(n = \mathbf{1}'x)\frac{\Pr(x \,|\, \lambda)}{\Pr(\mathbf{1}'x = n \,|\, \lambda)} \ .
\end{aligned}
$$

The following results state important properties of the Multinomial distribution. The proof of these properties is simple, using the characterization of the Multinomial by the Poisson, and the Poisson reproductive property.

Theorem 5: Multinomial Class Partition

Let $1\!:\!m$ be the index domain for the classes of a order m Multinomial distribution. Let T be a partition matrix breaking the m-classes into s-super-classes. Let $x \sim \mathrm{Mn}_m(n, \theta)$, then $y = Tx \sim \mathrm{Mn}_s(n, T\theta)$.

Theorem 6: Multinomial Conditioning on the Partial Sum.

If $x \sim \mathrm{Mn}_m(n, \theta)$, then the distribution of part of the vector x conditioned on its sum has Multinomial distribution, having as parameter the corresponding part of the original (normalized) parameters. In more detail, conditioning on the t first components, we have:

$$x_{1:t} \,|\, (\mathbf{1}'x_{1:t} = j) \sim \mathrm{Mn}_t\left(j, \frac{1}{\mathbf{1}'\theta_{1:t}}\theta_{1:t}\right) \text{ where } 0 \leq j \leq n \ .$$

Theorem 7: Multinomial–Binomial Decomposition.

Using the last two theorems, if $x \sim \mathrm{Mn}_m(n, \theta)$,

$$
\begin{aligned}
\Pr(x \,|\, n, \theta) \;=\; &\sum_{j=0}^{n} \Pr\left(x_{1:t} \,|\, j, \frac{1}{\mathbf{1}'\theta_{1:t}}\theta_{1:t}\right) \\
&\Pr\left(x_{t+1:m} \,|\, (n-j), \frac{1}{\mathbf{1}'\theta_{t+1:m}}\theta_{t+1:m}\right) \\
&\Pr\left(\begin{bmatrix} j \\ (n-j) \end{bmatrix} \,\Big|\, n, \begin{bmatrix} \mathbf{1}'\theta_{1:t} \\ \mathbf{1}'\theta_{t+1:m} \end{bmatrix}\right) \ .
\end{aligned}
$$

Analogously, we could write the Multinomial-Trinomial decomposition for a three-partition of the class indices in three super-classes. More generally, we could also write the m-nomial-s-nomial decomposition for the partition of the m class indices into s super-classes.

B.4 Multivariate Hypergeometric Distribution

In the first section we have shown how an Hypergeometric variate can be generated from a Bernoulli process. The natural generalization of this result is obtained considering a Multinomial process. As in the last section, we say that u^i is of class k, $c(u^i) = k$, iff $u^i = I^k$.

We take a sample of size n from a finite population of size $N(> n)$, that is partitioned into m classes. The population frequencies (number of elements in each category) are represented by $[\psi_1, \ldots \psi_m]$, hence $N = \mathbf{1}'\psi$. Based on the sample, we want to make an inference on ψ. x_k é is the sample frequency of class k.

One way of describing this problem is to consider an urn with N balls of m different colors, indexed by $1, \ldots m$. ψ_k is the number of balls of color k. Assume that the N balls are separated into two smaller boxes, so that box 1 has n balls and box 2 has the remaining $N - n$ balls. The statistician can observe the composition of box 1, represented by vector x of sample frequencies. The quantity of interest for the statistician is the vector $\psi - x$ representing the composition of box 2.

As in the bivariate case, we assume that $U^{1:N}$ is a finite sub-sequence in an exchangeable process and, therefore, any sub-sequence extracted from $U^{1:N}$ has the same distribution of $U^{1:n}$. Hence, $x = U^{1:n}\mathbf{1}$ has the same distribution of the frequency vector for a sample of size n.

As in the bivariate case, our objective is to find the distribution of $x \,|\, \psi$. Again, using de Finetti theorem, there is a vector $\mathbf{0} \le \theta \le \mathbf{1}$, $\mathbf{1}'\theta = 1$, such that $\coprod_{j=0}^{N} u^j \,|\, \theta$ and $\Pr\left(c(u^j) = k\right) = \theta_k$.

Theorem 8: As in the Multinomial case, the following results follow:

- $\psi \,|\, \theta \sim \mathrm{Mn}_m(N, \theta)$;

- $x \,|\, \theta \sim \mathrm{Mn}_m(n, \theta)$;

- $(\psi - x) \,|\, \theta \sim \mathrm{Mn}_m((N - n), \theta)$;

- $(\psi - x) \amalg x \,|\, \theta$.

Using the results of the last section and following the same steps as in the Hy_2 case in the first section, we obtain the following expression for m-variate Hypergeometric

distribution, $x^n \,|\, [n, N, \psi] \sim \mathrm{Hy}_m(n, N, \psi)$:

$$\Pr(x^n \,|\, n, \psi) = \frac{\dbinom{n}{x^n} \dbinom{N-n}{\psi - x^n}}{\dbinom{N}{\psi}}$$

where $\mathbf{0} \le x^n \le \psi \le N\mathbf{1}$, $\mathbf{1}'x^n = n$, $\mathbf{1}'\psi = N$.

This is the vector representation of the Hypergeometric probability distribution.

$$x^n \,|\, [n, x^N] \sim \mathrm{Hy}(n, N, x^N) .$$

Alternatively, we can write the more usual formula,

$$\Pr(x \,|\, \psi) = \frac{\dbinom{\psi_1}{x_1} \dbinom{\psi_2}{x_2} \cdots \dbinom{\psi_m}{x_m}}{\dbinom{N}{n}} .$$

Theorem 9: The expectation and covariance of a random vector with Hypergeometric distribution, $x \sim \mathrm{Hy}_m(n, N, \psi)$, are:

$$\mathrm{E}(x) = n\widetilde{\psi} , \quad \mathrm{Cov}(x) = n\frac{N-n}{N-1}\left(\mathrm{diag}(\widetilde{\psi}) - \widetilde{\psi} \otimes \widetilde{\psi}'\right) \text{ where } \widetilde{\psi} = \frac{1}{N}\psi .$$

Proof: Use that

$$
\begin{aligned}
\mathrm{Cov}(x^n) &= n\mathrm{Cov}(u^1) + n(n-1)\mathrm{Cov}(u^1, u^2)\\
\mathrm{Cov}(u^1) &= \mathrm{E}\left(u^1 \otimes (u^1)'\right) - \mathrm{E}(u^1) \otimes \mathrm{E}(u^1)' = \mathrm{diag}(\widetilde{\psi}) - \widetilde{\psi} \otimes \widetilde{\psi}'\\
\mathrm{Cov}(u^1, u^2) &= \mathrm{E}\left(u^1 \otimes (u^2)'\right) - \mathrm{E}(u^1) \otimes \mathrm{E}(u^2)' .
\end{aligned}
$$

The second term of the last two equations are equal, and the first term of the last equation is

$$\mathrm{E}\left(u_i^1 u_j^2\right) = \begin{cases} \frac{\psi_i}{N}\frac{\psi_i - 1}{N-1} & \text{if } i = j \\ \frac{\psi_i}{N}\frac{\psi_j}{N-1} & \text{if } i \ne j \end{cases}$$

Algebraic manipulation yields the result.

Note that, as in the order 2 case, the diagonal elements of $\mathrm{Cov}(u^1)$ are positive, while the diagonal elements of $\mathrm{Cov}(u^1, u^2)$ are negative. In the off diagonal elements, the signs are reversed.

B.5 Dirichlet Distribution

In the second section we presented the multinomial distribution, $\mathrm{Mn}_m(n, \theta)$. In this section we present the Dirichlet distribution for the parameter θ. Let us first recall the univariate Poisson and Gamma distributions.

A random variable has Gamma distribution, $x \,|\, [a, b] \sim G(a, b), a, b > 0$, if its distribution is continuous with density

$$f(x \,|\, a, b) = \frac{b^a}{\Gamma(a)} x^{a-1} \exp(-bx) \ , \ x > 0 \ .$$

The expectation and variance of this variate are

$$E(x) = \frac{a}{b} \ \text{and} \ \mathrm{Var}(x) = \frac{a}{b^2} \ .$$

Lemma 10: Reproductive property for the Gamma distribution.
If n independent random variables $x_i \,|\, a_i, b \sim G(a_i, b)$, then

$$\mathbf{1}'x \sim G(\mathbf{1}'a, b) \ .$$

Lemma 11: The Gamma distribution is conjugate to the Poisson distribution.

Proof:
If $y \,|\, \lambda \sim \mathrm{Ps}(\lambda)$ and λ has prior $\lambda \,|\, a, b \sim G(a, b)$, then

$$\begin{aligned}
f(\lambda \,|\, y, a, b) \ &\propto \ L(\lambda \,|\, y)f(\lambda) \\
&= \ \exp(-\lambda)\frac{\lambda^y}{y!} \ \frac{b^a}{\Gamma(a)} \lambda^{a-1} \exp(-b\lambda) \ \propto \ \lambda^{y+a-1} exp(-(b+1)\lambda) \ .
\end{aligned}$$

That is, the posterior distribution of λ is Gamma with parameters $[a + y, b + 1]$.

Definition: Dirichlet distribution.
A random vector

$$y \in \mathcal{S}_{m-1} \equiv \{y \in R^m \,|\, \mathbf{0} \le y \le \mathbf{1} \wedge \mathbf{1}'y = 1\}$$

has Dirichlet distribution of order m with positive $a \in R^m$ if its density is

$$\Pr(y \,|\, a) = \frac{y \triangle (a - \mathbf{1})}{B(a)} \ .$$

Note that $\mathcal{S}_{m-1}$, the $m - 1$ dimensional Simplex, is the region of R^m subject to the "constraint", $\mathbf{1}'y = 1$. Hence, a point in the Simplex has only $m - 1$ "degrees of freedom". In this sense we say that the Direchlet distribution has a "singular" representation. It is possible to give a non-singular representation to the distribution $[y_1, \ldots y_{m-1}]'$, known

as the Multivariate Beta distribution, but at the cost of obtaining a convoluted algebraic formulation that also loses the natural geometric interpretation of the singular form.

The normalization factor for the Dirichlet distribution is

$$B(a) \equiv \int_{y \in \mathcal{S}_{m-1}} (y \triangle (a-1))\, dy \ .$$

Lemma 12: Beta function.
The normalization factor for the Dirichlet distribution defined above is the Beta function, defined as

$$B(a) = \frac{\prod_{k=1}^{m} \Gamma(a_k)}{\Gamma(\mathbf{1}'a)} \ .$$

The proof is given at the end of this section.

Theorem 13: Dirichlet as Conjugate of the Multinomial:
If $\theta \sim \mathrm{Di}_m(a)$ and $x \mid \theta \sim \mathrm{Mn}_m(n, \theta)$ then

$$\theta \mid x \sim \mathrm{Di}_m(a + x) \ .$$

Proof:

We only have to remember that the Multinomial likelihood is proportional to $\theta \triangle x$, and that a Dirichlet prior is proportional to $\theta \triangle (a - \mathbf{1})$. Hence, the posterior is proportional to $\theta \triangle (x + a - 1)$. At the other hand, $B(a + x)$ is the normalization factor, i.e., equal to the integral on θ of $\theta \triangle (x + a - 1)$, and so we have a Dirichlet density function, as defined above.

Lemma 14: Dirichlet Moments.
If $\theta \sim \mathrm{Di}_m(a)$ and $p \in I\!\!N^m$, then

$$\mathrm{E}\,(\theta \triangle p) \;=\; \frac{B(a + p)}{B(a)} \ .$$

Proof:

$$\int_{\Theta} (\theta \triangle p) f(\theta \mid a) d\theta = \frac{1}{B(a)} \int_{\Theta} (\theta \triangle p)\,(\theta \triangle (a-1))\, d\theta =$$

$$\frac{1}{B(a)} \int_{\Theta} (\theta \triangle (a + p - 1))\, d\theta \;=\; \frac{B(a + p)}{B(a)} \ .$$

Choosing the exponents, p, appropriately, we have

Corollary 15: If $\theta \sim \mathrm{Di}_m(a)$, then

$$
\begin{aligned}
\mathrm{E}(\theta) &= \tilde{a} \equiv \frac{1}{\mathbf{1}'a}a \\
\mathrm{Cov}(\theta) &= \frac{1}{\mathbf{1}'a+1}\left(\mathrm{diag}(\tilde{a}) - \tilde{a}\otimes\tilde{a}'\right) .
\end{aligned}
$$

Theorem 16: Characterization of the Dirichlet by the Gamma:
Let the components of the random vector $x \in R^m$ be independent variables with distribution $G(a_k, b)$. Then, the normalized vector

$$
y = \frac{1}{\mathbf{1}'x}x \sim \mathrm{Di}_m(a) , \ \ \mathbf{1}'x \sim \mathrm{Ga}(\mathbf{1}'a) \text{ and } y \amalg \mathbf{1}'x .
$$

Proof:

Consider the normalization,

$$
y = \frac{1}{t}x , \ \ t = \mathbf{1}'x , \ \ x = ty ,
$$

as a transformation of variables. Note that one of the new variables, say $y_m \equiv t(1 - y_1 \ldots - y_{m-1})$, becomes redundant.

The Jacobian matrix of this transformation is

$$
J = \frac{\partial\left(x_1, x_2, \ldots x_{m-1}, x_m\right)}{\partial\left(y_1, y_2, \ldots y_{m-1}, t\right)} = \begin{bmatrix}
t & 0 & \cdots & 0 & y_1 \\
0 & t & \cdots & 0 & y_2 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & t & y_{m-1} \\
-t & -t & \cdots & -t & 1 - y_1 \cdots - y_{m-1}
\end{bmatrix} .
$$

By elementary operations (see appendix F) that add all rows to the last one, we obtain the LU factorization the Jacobian matrix, $J = LU$, where

$$
L = \begin{bmatrix}
1 & 0 & \cdots & 0 & 0 \\
0 & 1 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 1 & 0 \\
-1 & -1 & \cdots & -1 & 1
\end{bmatrix} \text{ and } U = \begin{bmatrix}
t & 0 & \cdots & 0 & y_1 \\
0 & t & \cdots & 0 & y_2 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & t & y_{m-1} \\
0 & 0 & \cdots & 0 & 1
\end{bmatrix} .
$$

A triangular matrix determinant is equal to the product of the elements in its main diagonal, hence $|J| = |L|\,|U| = 1\,t^{m-1}$.

At the other hand, the joint distribution of x is

$$f(x) = \prod_{k=1}^{m} \text{Ga}(x_k \mid a_k, b) = \prod_{k=1}^{m} \frac{b^{a_k}}{\Gamma(a_k)} e^{-bx_k} (x_k)^{a_k - 1} \ .$$

and the joint distribution in the new system of coordinates is

$$g([y, t]) = |J| \, f\left(x^{-1}([y, t])\right)$$

$$= \ t^{m-1} \prod_{k=1}^{m} \frac{b^{a_k}}{\Gamma(a_k)} e^{-bx_k} (x_k)^{a_k - 1} \ = \ t^{m-1} \prod_{k=1}^{m} \frac{b^{a_k}}{\Gamma(a_k)} e^{-bty_k} (ty_k)^{a_k - 1}$$

$$= \ \left(\prod_{k=1}^{m} \frac{(y_k)^{a_k - 1}}{\Gamma(a_k)}\right) b^{\mathbf{1}'a} e^{-bt} t^{\mathbf{1}'a - m} t^{m-1} \ = \ \left(\prod_{k=1}^{m} \frac{(y_k)^{a_k - 1}}{\Gamma(a_k)}\right) b^{\mathbf{1}'a} e^{-bt} t^{\mathbf{1}'a - 1} \ .$$

Hence, the marginal distribution of $y = [y_1, \dots y_k]'$ is

$$g(y) = \int_{t=0}^{\infty} g([y, t]) dt$$

$$= \ \left(\prod_{k=1}^{m} \frac{(y_k)^{a_k - 1}}{\Gamma(a_k)}\right) \int_{t=0}^{\infty} b^{\mathbf{1}'a} e^{-bt} t^{\mathbf{1}'a - 1} dt$$

$$= \ \left(\prod_{k=1}^{m} \frac{(y_k)^{a_k - 1}}{\Gamma(a_k)}\right) \Gamma(\mathbf{1}'a) \ = \ \frac{y \triangle (a - 1)}{B(a)} \ .$$

In the last passage, we have replaced the integral by the normalization factor of a Gamma density, $\text{Ga}(\mathbf{1}'a, b)$. Hence, we obtain a density proportional to $y \triangle (a-1)$, i.e., a Dirichlet, Q.E.D.

In the last passage we also obtain the Dirichlet normalization factor, prooving the Beta function lemma.

Lemma 17: Bipartition of Indices for the Dirichlet.
Let $1\!:\!t$, $t\!+\!1\!:\!m$ be a bipartition of the class index domain, $1\!:\!m$, of an order m Dirichlet, in two super-classes. Let $y \sim \text{Di}_m(a)$, and

$$z^1 = \frac{1}{\mathbf{1}'y_{1:t}} y_{1:t} \ , \ \ z^2 = \frac{1}{\mathbf{1}'y_{t+1:m}} y_{t+1:m} \ , \ \ w = \left[\begin{array}{c} \mathbf{1}'y_{1:t} \\ \mathbf{1}'y_{t+1:m} \end{array} \right] \ .$$

We than have, $z^1 \amalg z^2 \amalg w$ and

$$z^1 \sim \text{Di}_t(a_{1:t}) \ , \ \ z^2 \sim \text{Di}_{m-t}(a_{t+1:m}) \text{ and } w \sim \text{Di}_2\left(\left[\begin{array}{c} \mathbf{1}'a_{1:t} \\ \mathbf{1}'a_{t+1:m} \end{array} \right]\right) \ .$$

Proof:

From the Dirichlet characterization by the Gamma we can imagine that the vector y is built by normalizing of a vector x, as follows,

$$y = \frac{1}{\mathbf{1}'x}x \ , \ \ x_k \sim \text{Ga}(a_k, b) \ , \ \ \prod_{k=1}^{m} x_k \ .$$

Considering isolatetly each one of the super-classes, we build the vectors z^1 and z^2 that are distributed as

$$\begin{aligned} z^1 &= \frac{1}{\mathbf{1}'y_{1:t}}y_{1:t} = \frac{1}{\mathbf{1}'x_{1:t}}x_{1:t} \sim \text{Di}_t(a_{1:t}) \\ z^2 &= \frac{1}{\mathbf{1}'y_{t+1:m}}y_{t+1:m} = \frac{1}{\mathbf{1}'x_{t+1:m}}x_{t+1:m} \sim \text{Di}_{m-t}(a_{t+1:m}) \ . \end{aligned}$$

$z^1 \text{ II } z^2$, that are in turn independent of the partial sums

$$\mathbf{1}'x_{1:t} \sim \text{Ga}(\mathbf{1}'a_{1:t}, b) \text{ and } \mathbf{1}'x_{t+1:m} \sim \text{Ga}(\mathbf{1}'a_{t+1:m}, b) \ .$$

Using again the theorem characterizing the Dirichlet by the Gamma distribution for these two Gamma variates, we obtain the result, Q.E.D.

We can generalize this result for any partition of the set of classes, as follows. If $y \sim \text{Di}_m(a)$ and T é is a s-partition of the m classes, the intra and extra super-class distributions are independent Dirichlets, as follows

$$\begin{aligned} z^r &= \frac{1}{T_r y} \, {_r}Py \sim \text{Di}_{T_r 1}\left({_r}Pa\right) \\ w &= Ty \sim \text{Di}_s(Ta) \ . \end{aligned}$$

B.6 Dirichlet-Multinomial

We say that a random vector $x \in I\!N^n \,|\, \mathbf{1}'x = n$ has Dirichlet-Multinomial (DM) distribution with parameters n and $a \in R^m$, iff

$$\Pr(x \,|\, n, a) = \frac{B(a+x)}{B(a)}\binom{n}{x} = \frac{B(a+x)}{B(a)\, B(x)}\frac{1}{x \triangle \mathbf{1}} \ .$$

Theorem 18: Characterization of the DM as a Dirichlet mixture of Multinomials.

$$\text{Se } \theta \sim \text{Di}_m(a) \text{ and } x \,|\, \theta \sim \text{Mn}(n, \theta) \text{ then } x \,|\, [n, a] \sim \text{DM}_m(n, a) \ .$$

Proof:

The joint distribution of θ, x is proportional to $\theta \bigtriangleup (a + x - 1)$, which integrated on θ is $B(a + x)$. Hence, multiplying by the joint distribution constants, we have the marginal for x, Q.E.D. Therefore, we have also proved that the function DM is normalized, that is

$$
\begin{aligned}
\Pr(x) &= \int_{\theta \in \mathcal{S}_{m-1}} \binom{n}{x} (\theta \bigtriangleup x) \frac{1}{B(a)} \theta \bigtriangleup (a - 1) \, d\theta \\
&= \frac{1}{B(a)} \binom{n}{x} \int_{\theta \in \mathcal{S}_{m-1}} (\theta \bigtriangleup (x + a - 1)) \, d\theta = \frac{B(x + a)}{B(a)} \binom{n}{x} .
\end{aligned}
$$

Theorem 19: Characterization of the DM by m Negative Binomials.
Let $a \in \mathbb{N}_+^m$, and $x \in \mathbb{N}_m$, be a vector whose components are independent random variables, $a_k \sim \mathrm{NB}(a_k, \theta)$. Then

$$
x \,|\, [\mathbf{1}'x = n, a] \sim \mathrm{DM}_m(n, a) .
$$

Proof:

$$
\Pr(x \,|\, \theta, a) = \prod_{k=1}^m \binom{a_k + x_k - 1}{x_k} \theta^{a_k} (1 - \theta)^{x_k}
$$

$$
\Pr(\mathbf{1}'x \,|\, \theta, a) = \binom{\mathbf{1}'a + \mathbf{1}'x - 1}{\mathbf{1}'x} \theta^{\mathbf{1}'a} (1 - \theta)^{\mathbf{1}'a} .
$$

Then,

$$
\Pr(x \,|\, \mathbf{1}'x = n, \theta, a) = \frac{\Pr(x \,|\, a, \theta)}{\Pr(\mathbf{1}'x = n \,|\, \theta)} = \frac{\prod_{k=1}^m \binom{a_k + x_k - 1}{x_k}}{\binom{\mathbf{1}'a + \mathbf{1}'x - 1}{\mathbf{1}'x}} .
$$

Hence,

$$
\begin{aligned}
\Pr(x \,|\, \mathbf{1}'x = n, \theta, a) &= \Pr(x \,|\, \mathbf{1}'x = n, a) \\
&= \prod_{k=1}^m \frac{\Gamma(a_k + x_k)}{x! \Gamma(a_k)} \Big/ \frac{\Gamma(\mathbf{1}'a + n)}{\Gamma(\mathbf{1}'a) n!} = \frac{B(a + x)}{B(a)} \binom{n}{x} .
\end{aligned}
$$

Theorem 20: The DM as Pseudo-Conjugate for the Hypergeometric

Se $x \sim \mathrm{Hy}_m(n, N, \psi)$ and $\psi \sim \mathrm{DM}_m(N, a)$ then $(\psi - x) \,|\, x \sim \mathrm{DM}_m(N - n, a)$.

Proof: Using the properties of the Hypergeometric already presented, we have the independence relation, $(\psi - x) \amalg x \,|\, \theta$. We can therefore use the Multinomial sample $x \,|\, \theta$ for updating the prior and obtain the posterior

$$
\theta \,|\, x \sim \mathrm{Di}_m(a + x) .
$$

Hence, the distribution of the non sampled pat of the population, $\psi - x$, given the sample x, is a mixture of $(\psi - x)\theta$ buy the posterior for θ. By the characterization of the DM as a mixture of Multinomials by a Dirichlet, the theorem follows, i.e.,

$$\left. \begin{array}{c} (\psi - x) \,|\, [\theta, x] \sim (\psi - x) \,|\, \theta \sim \mathrm{Mn}_m(N - n, \theta) \\ \theta \,|\, x \sim \mathrm{Di}_m(a + x) \end{array} \right\} \Rightarrow$$

$$\Rightarrow (\psi - x) \,|\, x \sim \mathrm{Di}_m(N - n, a + x) \ .$$

Lemma 21: DM Expectation and Covariance.
If $\ x \sim \mathrm{DM}_m(n, a)\ $ then

$$\begin{aligned} \mathrm{E}(x) &= n\widetilde{a} \equiv \frac{1}{\mathbf{1}'a}a \\ \mathrm{Cov}(x) &= \frac{n(n + \mathbf{1}'a)}{\mathbf{1}'a + 1} \left(\mathrm{diag}(\widetilde{a}) - \widetilde{a} \otimes \widetilde{a}' \right) \ . \end{aligned}$$

Proof:

$$\begin{aligned} \mathrm{E}(x) &= \mathrm{E}_\theta \left(\mathrm{E}_x(x \,|\, \theta) \right) = \mathrm{E}_\theta(n\theta) = n\widetilde{a} \\ \mathrm{E}(x \otimes x') &= \mathrm{E}_\theta \left(\mathrm{E}_x(x \otimes x' \,|\, \theta) \right) \\ &= \mathrm{E}_\theta \left(\mathrm{E}(x \,|\, \theta) \otimes \mathrm{E}(x \,|\, \theta)' + \mathrm{Cov}(x \,|\, \theta) \right) \\ &= \mathrm{E}_\theta \left(n \left(\mathrm{diag}(\theta) - \theta \otimes \theta' \right) + n^2 \theta \otimes \theta' \right) \\ &= n \, \mathrm{E}_\theta \left(\mathrm{diag}(\theta) \right) + n(n - 1) \, \mathrm{E}_\theta(\theta \otimes \theta') \\ &= n\mathrm{diag}(\widetilde{a}) + n(n - 1) \left(\mathrm{E}(\theta) \otimes \mathrm{E}(\theta)' + \mathrm{Cov}(\theta) \right) \\ &= n\mathrm{diag}(\widetilde{a}) + n(n - 1) \left(\widetilde{a} \otimes \widetilde{a}' + \frac{1}{\mathbf{1}'a + 1} \left(\mathrm{diag}(\widetilde{a}) - \widetilde{a} \otimes \widetilde{a}' \right) \right) \\ &= n\mathrm{diag}(\widetilde{a}) + n(n - 1) \left(\frac{1}{\mathbf{1}'a + 1}\mathrm{diag}(\widetilde{a}) + \frac{\mathbf{1}'a}{\mathbf{1}'a + 1}\widetilde{a} \otimes \widetilde{a}' \right) \\ \mathrm{Cov}(x) &= \mathrm{E}(x \otimes x') - \mathrm{E}(x) \otimes \mathrm{E}(x)' = \mathrm{E}(x \otimes x') - n^2\widetilde{a} \otimes \widetilde{a}' \\ &= \left(n + \frac{n(n - 1)}{\mathbf{1}'a + 1} \right) \mathrm{diag}(\widetilde{a}) + \left(n(n - 1)\frac{\mathbf{1}'a}{\mathbf{1}'a + 1} - n^2 \right) \widetilde{a} \otimes \widetilde{a}' \\ &= \frac{n(n + \mathbf{1}'a)}{\mathbf{1}'a + 1} \left(\mathrm{diag}(\widetilde{a}) - \widetilde{a} \otimes \widetilde{a}' \right) \quad \text{Q.E.D.} \end{aligned}$$

Theorem 22: DM Class Bipartition
Let $1:t$, $t + 1:m$ a bipartition of the index domain for the classes of an order m DM, $1:m$, in two super-classes. Then, the following conditions (i) to (iii) are equivalent to condition (iv):

i: $x_{1:t} \amalg x_{t+1:m} \,|\, n_1 = \mathbf{1}'x_{1:t}$;

ii-1: $x_{1:t} \,|\, n_1 = \mathbf{1}'x_{1;t} \sim \mathrm{DM}_t(n_1, a_{1:t})$;

ii-2: $x_{t+1:m} \,|\, n_2 = \mathbf{1}' x_{t+1:m} \sim \mathrm{DM}_{m-t}(n_2, a_{t+1:m})$;

iii: $\begin{bmatrix} n_1 \\ n_2 \end{bmatrix} \sim \mathrm{DM}_2 \left(n, \begin{bmatrix} \mathbf{1}' a_{1:t} \\ \mathbf{1}' a_{t+1:m} \end{bmatrix} \right)$;

iv: $x \sim \mathrm{DM}_m(n, a)$.

Proof: We only have to show that the joint distribution can be factored in this form. By the DM characterization as a mixture, we can write it as Dirichlet mixture of Multinomials. By the bipartition theorems, we can factor both, the Multinomials and the Dirichlet, so the theorem follows.

B.7   Dirichlet of the Second Kind

Consider $y \sim \mathrm{Di}_{m+1}(a)$. The vector $z = (1/y_{m+1})y_{1:m}$ has Dirichlet of the Second Kind (D2K) distribution.

Theorem 23: Characterization of D2K by the Gamma distribution.
Using the characterization of the Dirichlet by the Gamma, we can write the D2K variate as a function of $m + 1$ independent Gamma variates,

$$z_{1:m} \sim (1/x_{m+1})x_{1:m} \quad \text{where} \quad x_k \sim Ga(a_k, b) .$$

Similar to what we did for the Dirichlet (of the first kind), we can write the D2K distribution and its moments as:

$$f(z \,|\, a) = \frac{z \triangle (a_{1:m} - 1)}{(1 + \mathbf{1}'z)^{\mathbf{1}'a} \, B(a)} ,$$

$$E(z) = e = (1/a_{m+1})a_{1:m} ,$$

$$\mathrm{Cov}(z) = \frac{1}{a_{m+1} - 2} \left(\mathrm{diag}(e) + e \otimes e' \right) .$$

The logarithm of a Gamma variate is well approximated by a Normal variate, see Aitchison & Shen (1980). This approximation is the key to several efficient computational procedures, and motivates the computation of the first two moments of the log-D2K distribution. For that, we use the Digamma, $\psi(\,)$, and Trigamma function, $\psi'(\,)$, defined as:

$$\psi(a) = \frac{d}{da} \ln \Gamma(a) = \frac{\Gamma'(a)}{\Gamma(a)} \ , \quad \psi'(a) = \frac{d}{da}\psi(a) .$$

Lemma 24: The expectation and covariance of a log-D2K variate are:

$$E(\log(z)) = \psi(a_{1:m}) - \psi(a_{m+1})\mathbf{1} ,$$

$$\text{Cov}(\log(z)) = \text{diag}\left(\psi'(a_{1:m})\right) + \psi'(a_{m+1})\mathbf{1} \otimes \mathbf{1}' \ .$$

Proof: Consider a Gamma variate, $x \sim G(a, 1)$:

$$1 = \int_0^\infty f(x)dx = \int_0^\infty \frac{1}{\Gamma(a)}x^{a-1}\exp(-x)dx \ .$$

Taking the derivative with respect to parameter a, we have

$$0 = \int_0^\infty \ln(x)x^{a-1}\frac{\exp(-x)}{\Gamma(a)}dx - \frac{\Gamma'(a)}{\Gamma^2(a)}\Gamma(a) = E(\ln(x)) - \psi(a) \ .$$

Taking the derivative with respect to parameter a a second time,

$$\begin{aligned}
\psi'(a) &= \frac{d}{da}E(\ln(x)) = \frac{d}{da}\int_0^\infty \frac{\ln(x)}{\Gamma(a)}x^{a-1}\exp(-x)dx \\
&= \int_0^\infty \ln(x)^2 x^{a-1}\frac{\exp(-x)}{\Gamma(a)}dx - \frac{\Gamma'(a)}{\Gamma(a)}E(\ln(x)) \\
&= E(\ln(x)^2) - E(\ln(x))^2 = \text{Var}(\ln(x)) \ .
\end{aligned}$$

The lemma follows from the D2K characterization by the Gamma.

B.8   Examples

Example 1: Let A, B be two attributes, each one of them present or absent in the elements of a population. Then each element of this population can be classified in exactly one of $2^2 = 4$ categories

A	B	k	I^k
present	present	1	$[1,0,0,0]'$
present	absent	2	$[0,1,0,0]'$
absent	present	3	$[0,0,1,0]'$
absent	absent	4	$[0,0,0,1]'$

According to the notation above, we can write $x \,|\, n, \theta \sim \text{Mn}_4(n, \theta)$.

If $\theta = [0.35,\ 0.20,\ 0.30,\ 0.15]$ and $n = 10$, then

$$\Pr(x^{10} \,|\, n, \theta) = \left(\begin{array}{c} 10 \\ x^{10} \end{array} \right)(\theta \triangle x^{10}) \ .$$

Hence, in order to compute the probability of $x = [1, 2, 3, 4]'$ given θ, we use the expression above, obtaining

$$\Pr\left(\begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \end{bmatrix} \,\middle|\, \begin{bmatrix} 0.35 \\ 0.20 \\ 0.30 \\ 0.15 \end{bmatrix} \right) = 0.000888 \ .$$

Example 2: If $X \mid \theta \sim \mathrm{Mn}_3(10, \theta)$, $\theta = [0.20,\ 0.30,\ 0.15]$, one can conclude, using the result above, that

$$\mathrm{E}(X) = (2, 3, 1.5) \ ,$$

while the covariance matrix is

$$\Sigma = \begin{bmatrix} 1.6 & -0.6 & -0.3 \\ -0.6 & 2.1 & -0.45 \\ -0.3 & -0.45 & 1.28 \end{bmatrix} \ .$$

Example 3: Assume that $X \mid \theta \sim \mathrm{Mn}_3(10, \theta)$, with $\theta = [0.20, 0.30, 0.15]$, as in Example 2. Let us take $A_0 = \{0, 1\}$, $A_1 = \{2, 3\}$. Then,

$$\sum_{A_1} X_i \mid \theta = X_2 + X_3 \mid \theta \sim \mathrm{Mn}_1(10, \theta_2 + \theta_3) \ ,$$

or

$$X_2 + X_3 \mid \theta \sim \mathrm{Mn}_1(10, 0.45) \ .$$

Analogously,

$$\begin{aligned} X_0 + X_1 \mid \theta &\sim \mathrm{Mn}_1(10, 0.55) \ , \\ X_1 + X_3 \mid \theta &\sim \mathrm{Mn}_1(10, 0.35) \ , \\ X_2 \mid \theta &\sim \mathrm{Mn}_1(10, 0.30) \ . \end{aligned}$$

Note that, in general, if $X \mid \theta \sim \mathrm{Mn}_k(n, \theta)$ then $X_i \mid \theta \sim \mathrm{Mn}_1(n, \theta_i)$, $i = 1, ..., k$.

Example 4: 3x3 Contingency Tables.

Assume that $X \mid \theta \sim \mathrm{Mn}_8(n, \theta)$, as in a 3x3 Contingency Tables:

x_{11}	x_{12}	x_{13}	$x_{1\bullet}$
x_{21}	x_{22}	x_{23}	$x_{2\bullet}$
x_{31}	x_{32}	x_{33}	$x_{3\bullet}$
$x_{\bullet 1}$	$x_{\bullet 2}$	$x_{\bullet 3}$	n

Applying Theorem 5 we get

$$(X_{1\bullet}, X_{2\bullet}) \mid \theta \sim \mathrm{Mn}_2(n, \theta'), \theta' = (\theta_{1\bullet}, \theta_{2\bullet}), \theta'_0 = \theta_3 \ .$$

This result tell us that

$$(X_{i1}, X_{i2}, X_{i3}) \mid \theta \sim \mathrm{Mn}_3(n, \theta'_i) \ ,$$

with

$$\theta'_i = (\theta_{i1}, \theta_{i2}, \theta_{i3}) \ , \quad \theta'_{0i} = 1 - \theta_{i\bullet} \ , \quad i = 1, 2, 3 \ .$$

We can now apply Theorem 6 to obtain the probability distribution of each row of the contingency table, conditioned on its sum, or conditioned on the sum of the other rows. We have

$$(X_{i1}, X_{i2}) \,|\, x_{i\bullet}\,, \theta \sim \mathrm{Mn}_2(x_{i\bullet}, \theta'_i)$$

with

$$\theta'_i = \frac{(\theta_{il}, \theta_{i2})}{\theta_{i\bullet}} \;,\; \theta'_{0i} = \frac{\theta_{i3}}{\theta_{i\bullet}} \;.$$

The next result expresses the distribution of $X \,|\, \theta$ in term of the conditional distributions, of each row of the table, in its sum, and in term of the distribution of these sums.

Proposition 25: If $X \,|\, \theta \sim \mathrm{Mn}_{r^2-1}(n, \theta)$, as in an $r \times r$, contingency table, then $P(X \,|\, \theta)$ can be written as

$$P(X \,|\, \theta) = \left[\prod_{i=1}^r P(X_{i1}, ..., X_{i,r-1} \,|\, x_{i\bullet}, \theta) \right] P(X_{1\bullet}, ..., X_{r-1\bullet} \,|\, \theta) \;.$$

Proof: We have:

$$
\begin{aligned}
P(X \,|\, \theta) &= n! \prod_{i=1}^r \frac{\theta_i^{x_i}}{x_i!} = n! \frac{\theta_{11}^{x_{11}} \; ... \; \theta_{rr}^{x_{rr}}}{x_{11}! \; ... \; x_{rr}!} \\
&= \left[\prod_{i=1}^r \frac{x_{i\bullet}!}{x_{i1}! \; ... \; x_{ir}!} \left(\frac{\theta_{i1}}{\theta_{i\bullet}} \right)^{x_{i1}} ... \left(\frac{\theta_{ir}}{\theta_{i\bullet}} \right)^{x_{ir}} \right] \frac{n!}{x_{i\bullet}! \; ... \; x_{r\bullet}!} \, \theta_{1\bullet}^{x_{1\bullet}} \; ... \; \theta_{r\bullet}^{x_{r\bullet}} \;.
\end{aligned}
$$

From Theorems 5 and 6, as in the last example, we recognize each of the first r factors above as the probabilities of each row in the table , conditioned on its sum, and recognize the last factor as the joint probability distribution of sum of these r rows.

Corollary 26: If $X \,|\, \theta \sim \mathrm{Mn}_{r^2-1}(n, \theta)$, as in Theorems 5 and 6, then

$$P(X \,|\, x_{1\bullet}, ..., x_{r-1\bullet}, \theta) = \prod_{i=1}^r P(X_{i1}, ..., X_{i,r-1} \,|\, x_{i\bullet}, \theta)$$

and, knowing $\theta, x_{1\bullet}, ..., x_{r-1\bullet}$,

$$(X_{11}, ..., X_{1,r-1}) \; \mathrm{II} \; ... \; \mathrm{II} \; (X_{r1}, ..., X_{r,r-1}) \;.$$

Proof: Since

$$P(X \mid \theta) = P(X \mid x_{1\bullet}, ..., x_{r-1\bullet}, \theta) P(X_{1\bullet}, X_{2\bullet}, ..., X_{r-1\bullet} \mid \theta) ,$$

from Theorems 5 and 6 we get the proposed equality.

The following result will be used next to express Theorem 7 as a canonical representation for $P(X \mid \theta)$.

Proposition 27: If $X \mid \theta \sim \mathrm{Mn}_{r^2-1}(n, \theta)$, as in Proposition, then a transformation

$$T : (\theta_{11}, ..., \theta_{1r}, ..., \theta_{r1}, ..., \theta_{r,r-1}) \rightarrow (\lambda_{11}, ..., \lambda_{1,r-1}, ..., \lambda_{r1}, ..., \lambda_{r,r-1}, \eta_1, ..., \eta_{r-1})$$

given by

$$\lambda_{11} = \frac{\theta_{11}}{\theta_{1\bullet}} \quad , \quad \cdots \quad , \quad \lambda_{1,r-1} = \frac{\theta_{1,r-1}}{\theta_{1\bullet}}$$

$$\vdots$$

$$\lambda_{r1} = \frac{\theta_{r1}}{\theta_{r\bullet}} \quad , \quad \cdots \quad , \quad \lambda_{r,r-1} = \frac{\theta_{r,r-1}}{\theta_{r\bullet}}$$

$$\eta_1 = \theta_{1\bullet}, \ \eta_2 = \theta_{2\bullet}, ..., \eta_{r-1} = \theta_{(r-1)\bullet}$$

is a onto transformation defined in $\{0 < \theta_{11} + ... + \theta_{r,r-1} < 1 \ ; \quad 0 < \theta ij < 1\}$ over the unitary cube of dimension $r^2 - 1$. Moreover, the Jacobian of this transformation, t, is

$$J = \eta^{r-1} \ \eta_1^{r-1} \ \cdots \ \eta_{r-1}^{r-1} \ (1 - \eta_1 - ... - \eta_{r-1})^{r-1} \ .$$

The proof is left as an exercise.

Example 5: Let us examine the case of a 2×2 contingency table:

x_{11}	x_{12}
x_{21}	x_{22}

n

θ_{11}	θ_{12}
θ_{21}	θ_{22}

1

In order to obtain the canonical representation of $P(X \mid \theta)$ we use the transformation T in the case $r = 2$:

$$\lambda_{11} = \frac{\theta_{11}}{\theta_{11} + \theta_{12}} ,$$

$$\lambda_{21} = \frac{\theta_{11}}{\theta_{21} + \theta_{22}} ,$$

$$\eta_1 = \theta_{11} + \theta_{12} ,$$

hence,

$$P(X \mid \theta) =$$

$$= \binom{x_{1\bullet}}{x_{11}} \lambda_{11}^{x_{11}} (1 - \lambda_{11})^{x_{12}} \binom{x_{2\bullet}}{x_{21}} \lambda_{21}^{x_{21}} (1 - \lambda_{21})^{x_{22}} \binom{n}{x_{1\bullet}} \eta_1^{x_{1\bullet}} (1 - \eta_1)^{x_{2\bullet}} ,$$

$$0 < \theta_{11} < 1 , \quad 0 < \theta_{21} < 1 , \quad 0 < \eta_1 < 1 .$$

B.9 Functional Characterizations

The objective of this section is to derive the general form of a homogeneous Markov random process. Theorem 28, by Reny and Aczel, states that such a process is described by a mixture of Poisson distributions. Our presentation follows Aczel (1966, sec. 2.1 and 2.3) and Janossy, Reny and Aczel (1950). It follows from the characterization of the Multinomial by the Poisson distribution given in theorem 4, that Reny-Aczel characterization of a homogeneous and local time point process is analogous to de Finetti characterization of an infinite exchangeable 0-1 process as a mixture of Bernoulli distributions, see for example Feller (1971, v.2, ch.VII, sec. 4).

Cauchy's Functional Equations

Cauchy's additive functional equation has the form

$$f(x + y) = f(x) + f(y) .$$

The following argument from Cauchy (1821) shows that a continuous solution of this functional equation must have the form

$$f(x) = cx .$$

Repeating the sum of the same argument, x, n times, we must have $f(nx) = nf(x)$. If $x = (m/n)t$, then $nx = mt$ and

$$nf(x) = f(nx) = f(mt) = mf(t) \text{ hence,}$$

$$f\left(\frac{m}{n}t\right) = \frac{m}{n}f(t) ,$$

taking $c = f(1)$, and $x = m/n$, it follows that $f(x) = cx$, over the rationals, $x \in \mathbb{Q}$. From the continuity condition for $f(x)$, the last result must also be valid over the reals, $x \in R$. Q.E.D.

Cauchy's multiplicative functional equation has the form

$$f(x + y) = f(x)f(y) , \quad \forall x, y > 0 , f(x) \geq 0 .$$

The trivial solution of this equation is $f(x) \equiv 0$. Assuming $f(x) > 0$, we take the logarithm, reducing the multiplicative equation to the additive equation,

$$\ln f(x_y) = \ln f(x) + \ln f(y) \ , \quad \text{hence,}$$

$$\ln f(x) = cx \ , \text{or} \ \ f(x) = \exp(cx) \ .$$

Homogeneous Discrete Markov Processes

We seek the general form of a homogeneous discrete Markov process. Let $w_k(t)$, for $t \geq 0$, be the probability of occurrence of exactly k events. Let us also assume the following hypotheses:

Time Locality: If $t_1 \leq t_2 \leq t_3 \leq t_4$ then, the number of events in $[t_1, t_2[$ is independents of the number of events in $[t_3, t_4[$.

Time Homogeneity: The distribution for the number of events occurring in $[t_1, t_2[$ depends only on the interval length, $t = t_2 - t_1$.

From time locality and homogeneity, we can decompose the occurrence of no (zero) events in $[0, t + u[$ as ,

$$w_0(t + u) = w_0(t) w_0(u) \ .$$

Hence, $w_0(t)$ must obey Cauchy's functional equation, and

$$w_0(t) = \exp(ct) = \exp(-\lambda t) \ .$$

Since $w_0(t)$ is a probability distribution, $w_0(t) \leq 1$, and $\lambda > 0$.

Hence, $v(t) = 1 - w_0(t) = 1 - \exp(-\lambda t)$, the probability of one or more events occurring before $t > 0$, must be the familiar exponential distribution.

For $k \geq 1$ occurrences before $t + u$, the general decomposition relation is

$$w_n(t + u) = \sum_{k=0}^{n} w_k(t) w_{n-k}(u) \ .$$

Theorem 28: (Reny-Aczel) The general (non trivial) solution of this this system of functional equations has the form:

$$w_k(t) = e^{-\lambda t} \sum_{<r,k>} \prod_{j=1}^{k} \frac{(c_j t)^{r_j}}{r_j!} \ , \quad \lambda = \sum_{j=1}^{\infty} c_j \ .$$

where the index set $< r, k, n >$ is defined as

$$< r, k, n >= \{r_1, r_2, \ldots r_k \,|\, r_1 + 2r_2 \ldots + kr_k = n\} \ .$$

and $< r, k >$ is a shorthand for $< r, k, k >$.

Proof. By induction: The theorem is true for $k = 0$. Let us assume, as induction hypothesis, that it is true to $k < n$. The last equation in the recursive system is

$$w_n(t + u) = \sum_{k=0}^{n} w_k(t) w_{n-k}(u) =$$

$$w_n(t) e^{-\lambda u} + w_n(u) e^{-\lambda t} + e^{-\lambda(t+u)} \sum_{k=1}^{n-1} \sum_{<r,k>} \sum_{<s,n-k>} \prod_{i=1}^{k} \frac{(c_i t)^{r_i}}{r_i!} \prod_{j=1}^{k} \frac{(c_j u)^{s_j}}{s_j!} .$$

Defining

$$f_n(t) = e^{\lambda t} w_n(t) - \sum_{<r,n-1,n>} \prod_{j=1}^{n-1} \frac{(c_j t)^{r_j}}{r_j!} ,$$

the recursive equation takes the form

$$f_n(t + u) = f_n(t) + f_n(u) ,$$

and can be solved as a general Cauchy's equation, that is,

$$f_n(t) = c_n t .$$

From the last equation and the definition of $f_n(t)$, we get the expression of $w_n(t)$ as in theorem 28. The constant λ is chosen so that the distribution is normalized.

The general solution given by theorem 28 represents a composition (mixture) of Poisson processes, where an event in the j-the process in the composition corresponds to the simultaneous occurrence of j single events in the original homogeneous Markov process. If we impose the following rarity condition, the general solution is reduced to a mixture of ordinary Poisson processes.

Rarity Condition: The probability that an event occurs in a short time at least once is approximately equal to the probability that it occurs exactly once, that is, the probability of simultaneous occurrences is zero.

B.10   Final Remarks

This work is in memory of Professor D Basu who was the supervisor of the first author PhD dissertation, the starting point for the research in Bayesian analysis of categorical data presented here. A long list of papers follows Basu and Pereira (1982). We have chosen a few that we recommend for additional reading: Albert (1985), Gunel (1984), Irony, Pereira and Tiwari (2000), Paulino and Pereira (1992, 1995) and Walker (1996). To make the analysis more realistic, extensions and mixtures of Dirichlet also were considered. For

instance see Albert and Gupta (1983), Carlson (1977), Dickey (1983), Dickey, Jiang and Kadane (1987), and Jiang, Kadane and Dickey (1992).

Usually the more complex distributions are used to realistic represent situations for which the strong properties of Dirichlet seems to be not realistic. For instance, in a 2 x 2 contingency table, the first line to be conditional independent of the second line given the marginal seems to be unrealistic in some situations. Mixtures of Dirichlet in some cases take care of the situation as shown by Albert and Gupta (1983).

The properties presented here are also important in non-parametric Bayesian statistics in order to understand the Dirichlet process for the competitive risk survival problem. See for instance Salinas-Torres, Pereira and Tiwari (1997, 2002). In order to be historically correct we cannot forget the important book of Wilks, published in 1962, where one can find the definition of Dirichlet distribution.

The material presented in this essay adopts a singular representation for several distributions, as in Pereira and Stern (2005). This representation is unusual in the statistical literature, but the singular representation makes it simpler to extend and generalize the results and greatly facilitates numerical and computational implementations.

We end this essay presenting the Reny-Aczel characterization of the Poisson mixture. This result can be interpreted as an alternative to de Finetti characterization theorem introduced in Finetti (1937). Using the characterization of binomial distributions by Poisson processes conditional arguments, as given by Theorem 4, and Blackwell (minimal) sufficiency properties discussed in Basu and Pereira (1983), Section 9 leads in fact to a De Finetti characterization for Binomial distributions. Also, if one recall the indifference principle (Mendel, 1989) the finite version of Finetti argument can simply be obtained. See also Irony and Pereira (1994) for the motivation of these arguments. The consideration of Section 9 could be viewed as a very simple formulation of the binomial distribution finite characterization.

Appendix C

Model Miscellanea

"Das Werdende, das ewig wirkt und lebt,
Umfass euch mit der Liebe holden Schranken,
Und was in schwankender Erscheinung schwebt,
Befestiget mit dauernden Gedanken!"

The becoming, which forever works and lives,
Holds you in love's gracious bonds,
And what fluctuates in apparent oscillations,
Fix it in place with enduring thoughts!

Johann Wolfgang von Goethe (1749-1832),
The Lord, in Faust, prologue in heaven.

"Randomness and order do not contradict each
other; more or less both may be true at once.
The randomness controls the world and due to
this in the world there is order and law, which
can be expressed in measures of random events
that follow the laws of probability theory."

Alfréd Rényi (1921 - 1970).

This appendix collects the material in some slide presentations on a miscellanea of statistical models used during the curse to illustrate several aspects of the FBST use and implementation. This appendix is not intended to be a self sufficient reading material, but rather a guide or further study. Section 1, on contingency table models, is (I hope) fully supplemented by the material on the Multinomial-Dirichlet distribution presented in appendix B. These models are of great practical importance, and also relatively simple

to implement and easy interpret. These characteristics make them ideal for the several statistical "experiments" required in the home works. Section 2, on a Wibull model, should require only minor additional reading, for further details see Barlow and Prochan (1981) and Ironi et al. (2002). This model highlights the importance of being able to incorporate expert opinion as prior information.

Sections 3 to 5, presenting several models based on the Normal-Wishard distribution, may require extensive additional readings. Some epistemological aspects of these models are discussed in chapters 4 and 5. The material in these sections is presented for completude, but its reading is optional, and only recommended for those students with a degree in statistics or equivalent knowledge. Of course, it is also possible to combine Normal-Wishad and Multinomial-Dirichlet models, in the form of mixture models, see section 6 and Lauretto and Stern (2005). Section 7 presents an overview of the REAL classification tree algorithm, for further details see Lauretto et al. (1998).

C.1   Contingency Table Models

Homogeneity test in 2×2 contingency table

This model is useful in many applications, like comparison of two communities with relation to a disease incidence, consumer behavior, electoral preference, etc. Two samples are taken from two binomial populations, and the objective is to test whether the success ratios are equal. Let x and y be the number of successes of two independent binomial experiments of sample sizes m and n, respectively. The posterior density for this multinomial model is,

$$f(\theta \mid x, y, n, m) \propto \theta_1^x \theta_2^{n-x} \theta_3^y \theta_4^{m-y}$$

The parameter space and the null hypothesis set are:

$$\Theta = \{0 \leq \theta \leq 1 \mid \theta_1 + \theta_2 = 1 \wedge \theta_3 + \theta_4 = 1\}$$

$$\Theta_0 = \{\theta \in \Theta \mid \theta_1 = \theta_3\}$$

The Bayes Factor considering a priori $Pr\{H\} = Pr\{\theta_1 = \theta_3\} = 0.5$ and uniform densities over Θ_0 and $\Theta - \Theta_0$ is given in the equation below. See [**?**] and [**?**] for details and discussion about properties.

$$BF = \frac{\binom{m}{x}\binom{n}{y}}{\binom{m+n}{x+y}} \frac{(m+1)(n+1)}{m+n+1}$$

Independence test in a 2×2 contingency table

Suppose that laboratory test is used to help in the diagnostic of a disease. It should be interesting to check if the test results are really related to the health conditions of a patient. A patient chosen from a clinic is classified as one of the four states of the set

$$\{(h, t) \mid h, t = 0 \text{ or } 1\}$$

in such a way that h is the indicator of the occurrence or not of the disease and t is the indicator for the laboratory test being positive or negative. For a sample of size n we record $(x_{00}, x_{01}, x_{10}, x_{11})$, the vector whose components are the sample frequency of each the possibilities of (t, h). The parameter space is the simplex

$$\Theta = \{(\theta_{00}, \theta_{01}, \theta_{10}, \theta_{11}) \mid \theta_{ij} \geq 0 \ \wedge \ \sum_{i,j} \theta_{ij} = 1\}$$

and the null hypothesis, h and t are independent, is defined by

$$\Theta_0 = \{\theta \in \Theta \mid \theta_{00} = \theta_{0\bullet}\theta_{\bullet 0}, \ \theta_{0\bullet} = \theta_{00} + \theta_{01}, \ \theta_{\bullet 0} = \theta_{00} + \theta_{10}\}.$$

The Bayes Factor for this case is discussed by [Iro 95] and has the following expression:

$$BF = \frac{\binom{x_{0\bullet}}{x_{00}}\binom{x_{1\bullet}}{x_{11}}}{\binom{n}{x_{\bullet 0}}} \left\{ \frac{(n+2)\{(n+3) - (n+2)[P(1-P) + Q(1-Q)]\}}{4(n+1)} \right\}$$

where $x_{i\bullet} = x_{i0} + x_{i1}, x_{\bullet j} = x_{0j} + x_{1j}$, $P = \frac{x_{0\bullet}}{n+2}$, and $Q = \frac{x_{\bullet 0}}{n+2}$.

C.2 Weibull Wearout Model

We where faced with the problem of testing the wearout of a lot of used display panels. A panel displays 12 to 18 characters. Each character is displayed as a 5×8 matrix of pixels, and each pixel is made of 2 (RG) or 3 (RGB) individual color elements, (like a light emitting diode or gas plasma device). A panel fails when the first individual color element fails. The construction characteristics of a display panel makes the weibull distribution specially well suited to model its life time. The color elements are "burned in" at the production process, so we assume they are not at the infant mortality region, i.e. we assume the Weibull's shape parameter to be greater than one, with wearout or increasing hazard rates.

The panels in question were purchased as used components, taken from surplus machines. The dealer informed the machines had been operated for a given time, and also

informed the mean life of the panels at those machines. Only working panels were acquired. The acquired panels were installed as components on machines of a different type. The use intensity of the panels at each type of machine corresponds to a different time scale, so mean lifes are not directly comparable. The shape parameter however is an intrinsic characteristic of the panel. The used time over mean life ratio, $\rho = \alpha/\mu$, is adimensional, and can therefore be used as an intrinsic measure of wearout. We have recorded the time to failure, or times of withdrawal with no failure, of the panels at the new machines, and want to use this data to corroborate (or not) the wearout information provided by the surplus equipment dealer.

Weibull Distribution

The two parameter Weibull probability density, reliability (or survival probability) and hazard functions, for a failure time $t \geq 0$, given the shape, and characteristic life (or scale) parameters, $\beta > 0$, and $\gamma > 0$, are:

$$
\begin{aligned}
w(t\,|\,\beta,\gamma) &= (\beta\,t^{\beta-1}/\gamma^{\beta})\,exp(-(t/\gamma)^{\beta}) \\
r(t\,|\,\beta,\gamma) &= exp(-(t/\gamma)^{\beta}) \\
z(t\,|\,\beta,\gamma) &\equiv w(\ )/r(\ ) = \beta\,t^{\beta-1}/\gamma^{\beta}
\end{aligned}
$$

The mean and variance of a Weibull variate are given by:

$$
\begin{aligned}
\mu &= \gamma\,\Gamma(1+1/\beta) \\
\sigma^2 &= \gamma^2(\Gamma(1+2/\beta) + \Gamma^2(1+1/\beta))
\end{aligned}
$$

By altering the parameter, β, $W(t\,|\,\beta,\gamma)$ takes a variety of shapes, Dodson(1994). Some values of shape parameter are important special cases: for $\beta = 1$, W is the exponential distribution; for $\beta = 2$, W is the Rayleigh distribution; for $\beta = 2.5$, W approximates the lognormal distribution; for $\beta = 3.6$, W approximates the normal distribution; and for $\beta = 5.0$, W approximates the peaked normal distribution. The flexibility of the Weibull distribution makes it very useful for empirical modeling, specially in quality control and reliability. The regions $\beta < 1$, $\beta = 1$, and $\beta > 1$ correspond to decreasing, constant and increasing hazard rates. These three regions are also known as infant mortality, memoryless, and wearout failures. γ is approximately the 63rd percentile of the life time, regardless of the shape parameter.

The Weibull also has important theoretical properties. If n i.i.d. random variables have Weibull distribution, $X_i \sim w(t\,|\,\beta,\gamma)$, then the first failure is a Weibull variate with characteristic life $\gamma/n^{1/\beta}$, i.e. $X_{[1,n]} \sim w(t\,|\,\beta,\gamma/n^{1/\beta})$. This kind of property allows a characterization of the Weibull as a limiting life distribution in the context of extreme value theory, Barlow and Prochan (1975).

The affine transformation $t = t' + \alpha$ leads to the three parameter truncated Weibull distribution. A location (or threshold) parameter, $\alpha > 0$ represents beginning observation of a (truncated) Weibull variate at $t = 0$, after it has already survived the period $[-\alpha, 0[$. The three parameter truncated Weibull is given by:

$$
\begin{aligned}
w(t \,|\, \alpha, \beta, \gamma) &= (\beta \,(t+\alpha)^{\beta-1}/\gamma^\beta)\, exp(-((t+\alpha)/\gamma)^\beta)/r(\alpha \,|\, \beta, \gamma) \\
r(t \,|\, \alpha, \beta, \gamma) &= exp(-((t+\alpha)/\gamma)^\beta)/r(\alpha \,|\, \beta, \gamma)
\end{aligned}
$$

Wearout Model

The problem described at the preceding sections can be tested using the FBST, with parameter space, hypothesis and posterior joint density:

$$
\begin{aligned}
\Theta &= \{(\alpha, \beta, \gamma) \in \,]0, \infty] \times [1, \infty] \times [0, \infty[\,\} \\
\Theta_0 &= \{(\alpha, \beta, \gamma) \in \Theta \,|\, \alpha = \rho\mu(\beta, \gamma) \,\} \\
f(\alpha, \beta, \gamma \,|\, D) &\propto \prod_{i=1}^{n} w(t_i \,|\, \alpha, \beta, \gamma) \prod_{j=1}^{m} r(t_j \,|\, \alpha, \beta, \gamma)
\end{aligned}
$$

where the data D are all the recorded failure times, $t_i > 0$, and the times of withdrawal with no failure, $t_j > 0$.

At the optimization step it is better, for numerical stability, to maximize the log-likelihood, $fl(\ )$. Given a sample with n recorded failures and m withdrawals,

$$
\begin{aligned}
wl_i &= \log(\beta) + (\beta - 1)\log(t_i + \alpha) - \beta\log(\gamma) - ((t_i + \alpha)/\gamma)^\beta + (\alpha/\gamma)^\beta \\
rl_j &= -((t_j + \alpha)/\gamma)^\beta + (\alpha/\gamma)^\beta \\
fl &= \sum_{i=1}^{n} wl_i + \sum_{j=1}^{m} rl_j
\end{aligned}
$$

the hypothesis being represented by the constraint

$$
h(\alpha, \beta, \gamma) = \rho\,\gamma\,\Gamma(1 + 1/\beta) - \alpha = 0
$$

The gradients of $fl(\ )$ and $h(\ )$ analytical expressions, to be given to the optimizer,

are:

$$dwl =$$
$$[\ (\beta - 1)/(t + \alpha) - ((t + \alpha)/\gamma)^\beta \beta/(t + \alpha) + (\alpha/\gamma)^\beta \beta/\alpha\,,$$
$$1/\beta + \log(t + \alpha) - \log(\gamma) - ((t + \alpha)/\gamma)^\beta \log((t + \alpha)/\gamma) + (\alpha/\gamma)^\beta \log(\alpha/\gamma)\,,$$
$$-\beta/\gamma + ((t + \alpha)/\gamma)^\beta \beta/\gamma - (\alpha/\gamma)^\beta \beta/\gamma\ ]$$

$$drl =$$
$$[\ -((t + \alpha)/\gamma)^\beta \beta/(t + \alpha) + (\alpha/\gamma)^\beta \beta/\alpha\,,$$
$$-((t + \alpha)/\gamma)^\beta \log((t + \alpha)/\gamma) + (\alpha/\gamma)^\beta \log(\alpha/\gamma)\,,$$
$$((t + \alpha)/\gamma)^\beta \beta/\gamma\,,\ -(\alpha/\gamma)^\beta \beta/\gamma\ ]$$

$$dh =$$
$$[\ -1\,,\ -\rho\,\gamma\,\Gamma'(1 + 1/\beta)\,\Gamma(1 + 1/\beta)/\beta^2\,,\ \rho\,\Gamma(1 + 1/\beta)\ ]$$

For gamma and digamma functions efficient algorithms see Spanier and Oldham (1987).

In this model, some prior distribution of the shape parameter is needed to stabilize the model. Knowing color elements' life time to be approximately normal, we consider $\beta \in [3.0, 4.0]$.

C.3   The Normal-Wishart Distribution

The matrix notation used in this section is defined in section F.1.

The Bayesian research group at IME-USP has developed several applications based on multidimensional normal models, including structure models, mixture models and factor analysis models. In this appendix we review the core theory of some of these models, since they are used in some of the illustrative examples in chapters 4 and 5. For implementation details, practical applications, case studies, and further comments, see Lauretto et al. (2003).

The conjugate family of priors for multivariate normal distributions is the Normal-Wishart family of distributions, DeGroot (1970). Consider the random matrix X with elements X_i^j , $i = 1 \ldots k$, $j = 1 \ldots n$, $n > k$, where each column, x^j, contains a sample vector from a k-multivariate normal distribution with parameters β (mean vector) and V (covariance matrix), or $R = V^{-1}$ (precision matrix).

Let $\bar{x}$ and W denote, respectively, the statistics:

$$\bar{x} = \frac{1}{n}\sum_{j=1}^{n}x^j = \frac{1}{n}X\mathbf{1}$$

$$W = \sum_{j=1}^{n}(x^j - \beta)(x^j - \beta)' = (X - \beta)(X - \beta)'$$

The random matrix W has Wishart distribution with n degrees of freedom and precision matrix R. The Normal and Wishart pdfs have the expressions:

$$f(\bar{x}\,|\,n,\beta,R) = (\frac{n}{2\pi})^{k/2}|R|^{1/2}\exp(-\frac{n}{2}(\bar{x}-\beta)'R(\bar{x}-\beta))$$

$$f(W\,|\,n,\beta,R) = c\,|W|^{(n-k-1)/2}\exp(-\frac{1}{2}\mathrm{tr}(W\,R))$$

$$c^{-1} = |R|^{-n/2}\,2^{nk/2}\,\pi^{k(k-1)/4}\prod_{j=1}^{k}\Gamma(\frac{n+1-j}{2})$$

Now consider the matrix X as above, with unknown mean β and unknown precision matrix R, and the statistic

$$S = \sum_{j=1}^{n}(x^j - \bar{x})(x^j - \bar{x})' = (X - \bar{x})(X - \bar{x})'$$

Taking as prior distribution for the precision matrix R the wishart distribution with $a > k - 1$ degrees of freedom and precision matrix $\dot{S}$ and, given R, taking as prior for β a multivariate normal with mean $\dot{\beta}$ and precision $\dot{n}R$, i.e.

$$p(\beta, R) = p(R)\,p(\beta\,|\,R)$$

$$p(R) \propto |R|^{(a-k-1)/2}\exp(-\frac{1}{2}\mathrm{tr}(R\,\dot{S}))$$

$$p(\beta\,|\,R) \propto |R|^{1/2}\exp(-\frac{\dot{n}}{2}(\beta-\dot{\beta})'R(\beta-\dot{\beta}))$$

The posterior distribution for the parameters β and R has the form:

$$p_n(\beta, R\,|\,n, \bar{x}, S) = p_n(R\,|\,n, \bar{x}, S)\,p_n(\beta\,|\,R, n, \bar{x}, S)$$

$$p_n(R\,|\,n, \bar{x}, S) \propto |R|^{(a+n-k-1)/2}\exp(-\frac{1}{2}\mathrm{tr}(R\,\ddot{S}))$$

$$p_n(\beta\,|\,R, n, \bar{x}, S) \propto |R|^{1/2}\exp(-\frac{\ddot{n}}{2}(\beta-\ddot{\beta})'R(\beta-\ddot{\beta}))$$

$$\ddot{\beta} = (n\bar{x}+\dot{n}\dot{\beta})/\ddot{n}\ ,\quad \ddot{n} = n+\dot{n}$$

$$\ddot{S} = S+\dot{S}+\frac{n\dot{n}}{n+\dot{n}}(\dot{\beta}-\bar{x})(\dot{\beta}-\bar{x})'$$

Hence, the posterior distribution for R is a Wishart distribution with $a + n$ degrees of freedom and precision $\ddot{S}$, and the conditional distribution for β, given R, is k-Normal with mean $\ddot{\beta}$ and precision $\ddot{n}R$. All covariance and precision matrices are supposed to be positive definite, $n > k$, $a > k - 1$, and $\dot{n} > 0$.

Non-informative improper priors are given by $\dot{n} = 0$, $\dot{\beta} = 0$, $a = 0$, $\dot{S} = 0$, i.e. we take a Wishart with 0 degrees of freedom as prior for R, and a constant prior for β, Box and Tiao (1973), DeGroot (1970), Zellner (1971). Then, the posterior for R is a Wishart with n degrees of freedom and precision S, and the posterior for β, given R, is k-Normal with mean $\bar{x}$ and precision nR.

We can now write the simplified log-posterior kernels:

$$
\begin{aligned}
fl(\beta, R \mid n, \bar{x}, S) &= fl(R \mid n, \bar{x}, S) + fl(\beta \mid R, n, \bar{x}, S) \\
fl(R \mid n, \bar{x}, S) = flr &= \frac{a + n - k - 1}{2} \log(|R|) - \frac{1}{2}\operatorname{tr}(R\,\ddot{S}) \\
fl(\beta \mid R, n, \bar{x}, S) = flb &= \frac{1}{2}\log(|R|) - \frac{\ddot{n}}{2}(\beta - \ddot{\beta})'R(\beta - \ddot{\beta})
\end{aligned}
$$

For the surprise kernel, relative to the uninformative prior, we only have to replace the factor $(a + n - k - 1)/2$ by $(a + n)/2$.

C.4   Structural Models

In this section we study the dose-equivalence hypothesis.

The dose-equivalence hypothesis, H, asserts a proportional response of a pair of response measurements to two different stimuli. The hypothesis also asserts proportional standard deviations, and equivalent correlations for each response pair. The proportionality coefficient, δ, is interpreted as the second stimulus dose equivalent to one unit of the first.

This can be seen as a simultaneous generalization of the linear mean structure, the linear covariance structure, and the Behrens-Fisher problems. The test proved to be useful when comparing levels of genetic expression, as well as to calibrate micro array equipment at BIOINFO, the genetic research task force at University of Sao Paulo. The application of the dose-equivalence model is similar to the much simpler bio-equivalence model used in pharmacology, and closely related by several other classic covariance structure models used in biology, psychology, and social sciences, as described in Anderson (1969), Bock and Bargnann (1966), Jiang and Sarkar (1998, 1999, 2000a,b), Jöreskog (1970), and McDonald (1962, 1974, 1975). We are not aware of any alternative test for the dose-equivalence hypothesis published in the literature.

C.4.1 Mean and Covariance Structure

As it is usual in the covariance structure literature, we will write $V(\gamma) = \sum \gamma_h G\{h\}$, where the matrices $G\{h\}$, $h = 1, \ldots k(k+1)/2$ form a basis for the space of $k \times k$ symmetric matrices; in our case, $k = 4$. The matrix notation is presented at Section F.1.

$$V(\gamma) = \sum_{h=1}^{10} \gamma_h G\{h\} = \begin{bmatrix} \gamma_1 & \gamma_5 & \gamma_7 & \gamma_8 \\ \gamma_5 & \gamma_2 & \gamma_9 & \gamma_{10} \\ \gamma_7 & \gamma_9 & \gamma_3 & \gamma_6 \\ \gamma_8 & \gamma_{10} & \gamma_6 & \gamma_4 \end{bmatrix} \ , \quad \text{where}$$

$$G\{h\} = \begin{bmatrix} \delta_h^1 & \delta_h^5 & \delta_h^7 & \delta_h^8 \\ \delta_h^5 & \delta_h^2 & \delta_h^9 & \delta_h^{10} \\ \delta_h^7 & \delta_h^9 & \delta_h^3 & \delta_h^6 \\ \delta_h^8 & \delta_h^{10} & \delta_h^6 & \delta_h^4 \end{bmatrix} \ ,$$

and the Kronecker-delta is $\delta_h^j = 1$ if $h = j$ and $\delta_h^j = 0$ if $h \neq j$.

The dose-equivalence hypothesis, H, asserts a proportional response of a pair of response measurements to two different stimuli. Each pair of response measurements is supposed to be a bivariate normal variate. H also asserts proportional standard deviations, and equivalent correlations for each pair of response measurements. The proportionality coefficient, δ, is interpreted as the dose, calibration or proportionality coefficient.

In order to get simpler expressions for the log-likelihood, the constraints and its gradients, we use in the numerical procedures an extended parameter space including the coefficient δ, and state the dose-equivalence optimization problem on the extended 15-dimensional space, with a 5-dimensional constraint:

$$\begin{aligned} \Theta &= \{\theta = [\gamma', \beta', \delta]' \in R^{10+4+1} \ , \ V(\gamma) > 0\} \\ \Theta_0 &= \{\theta \in \Theta \,|\, h(\theta) = 0\} \\ h(\theta) &= \begin{bmatrix} \delta^2 \gamma_1 - \gamma_3 \\ \delta^2 \gamma_2 - \gamma_4 \\ \delta^2 \gamma_5 - \gamma_6 \\ \delta \beta_1 - \beta_3 \\ \delta \beta_2 - \beta_4 \end{bmatrix} \end{aligned}$$

In order to be able to compute some gradients needed in the next section, we recall some matrix derivative identities, see Anderson (1969), Harville (1997), McDonald and Swaminathan (1973), Rogers (1980). We use $V = V(\gamma)$, $R = V^{-1}$, and C for a constant matrix.

$$\frac{\partial V}{\partial \gamma_h} = G\{h\} \ , \qquad \frac{\partial R}{\partial \gamma_h} = -R\,G\{h\}\,R \ ,$$

$$\frac{\partial \beta' C \beta}{\partial \beta} = 2\,C\,\beta \ , \qquad \frac{\partial \log(|V|)}{\partial \gamma_h} = \text{tr}(R\,G\{h\}) \ ,$$

$$\frac{\partial \ \text{frob2}(V - C)}{\partial \gamma_h} = 2 \sum_{i,j} (V - C) \odot G\{h\} \ .$$

We also define the auxiliary matrices:

$$P\{h\} = R \, G\{h\} \ , \qquad Q\{h\} = P\{h\} \, R \ .$$

C.4.2   Numerical Optimization

To find θ^* we use an objective function, to be minimized on the extended parameter space, given by a centralization term minus the log-posterior kernel,

$$
\begin{aligned}
f(\theta \,|\, n, \bar{x}, S) \ &= \ c \, n \, \text{frob2}(V - C) - flr - flb \\
&= \ c \, n \, \text{frob2}(V - C) - \frac{a + n - k}{2} \log(|R|) \\
&\quad + \frac{1}{2} \text{tr}(R \, \ddot{S}) + \frac{\ddot{n}}{2} (\beta - \ddot{\beta})' R (\beta - \ddot{\beta})
\end{aligned}
$$

Large enough centralization factors, c, times the squared Frobenius norm of $(V - C)$, where C are intermediate approximations of the constrained minimum, make the first points of the optimization sequence remain in the neighborhood of the empirical covariance (the initial C). As the optimization proceeds, we relax the centralization factor, i.e. make $c \to 0$, and maximize the pure posterior function. This is a standard optimization procedure following the regularization strategy of Proximal-Point algorithms, see Bertzekas and Tsitsiklis (1989), Iusem (1995), Censor and Zenios (1997). In practice this strategy let us avoid handling explicitly the difficult constraint $V(\gamma) > 0$.

Using the matrix derivatives given in the last section, we find the objective function's gradient, $\partial f / \partial \theta$,

$$
\begin{aligned}
\frac{\partial f}{\partial \gamma_h} \ &= \ \frac{a + n - k}{2} \text{tr}(P\{h\}) - \frac{1}{2} \text{tr}(Q\{h\} \, \ddot{S}) \\
&\quad - \frac{\ddot{n}}{2} (\beta - \ddot{\beta})' \, Q\{h\} \, (\beta - \ddot{\beta}) \\
&\quad + 2 c \, n \sum_{i,j=1}^{n} (V - C) \odot G\{h\} \\
\frac{\partial f}{\partial \beta} \ &= \ \ddot{n} \, R \, (\beta - \ddot{\beta})
\end{aligned}
$$

For the surprise kernel and its gradient, relative to the uninformative prior, we only have to replace the factor $(a + n - k)/2$ by $(a + n + 1)/2$.

The Jacobian matrix of the constraints, $\partial h/\partial\theta$, is:

$$
\begin{bmatrix}
\delta^2 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2\delta\gamma_1 \\
0 & \delta^2 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2\delta\gamma_2 \\
0 & 0 & 0 & 0 & \delta^2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2\delta\gamma_5 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \delta & 0 & -1 & 0 & \beta_1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \delta & 0 & 0 & -1 & \beta_2
\end{bmatrix}
$$

At the optimization step, Variable-Metric Proximal-Point algorithms, working with the explicit analytical derivatives given above, proved to be very stable, in contrast with the often unpredictable behavior of some methods found in most statistical software, like Newton-Raphson or "Scoring". Optimization problems of small dimension, like above, allow us to use dense matrix representation without significant loss, Stern (1994).

In order to handle several other structural hypotheses, we only have to replace the constraint, and its Jacobian, passed to the optimizer. Hence, many different hypothesis about the mean and covariance or correlation structure can be treated in a coherent, efficient, exact, robust, simple, and unified way.

The derivation of the Monte Carlo procedure for the numerical integrations required to implement the FBST in this model is presented in appendix G.

C.5 Factor Analysis

This section reviews the most basic facts about FA models. For a synthetic introduction to factor analysis, see Ghaharamani and Hilton (1997) and Everitt (1984). For some of the matrix analytic and algorithmic details, see Abadir and Magnus (2005), Golub and Loan (1989), Harville (2000), Rubin and Thayer (1982), and Russel (1998). For the technical issue of factor rotation, see Browne (1974, 2001), Jennrich (2001, 2002, 2004) and Bernaards and Jennrich (2005).

The generative model for Factor Analysis (FA) is $x = \Lambda z + u$, where x is a $p \times 1$ vector of observed random variables, z is a $k \times 1$ vector or latent (unobserved) random variables, known as *factors* and Λ is the $p \times k$ matrix of factor *loadings*, or weights. FA is used as a dimensionality reduction technique, so $k < p$.

The vector variates z and u are assumed to be distributed as $\mathcal{N}(0, I)$ and $\mathcal{N}(0, \Psi)$, where Ψ is diagonal. Hence, the observed and latent variables joint distribution is

$$
\begin{bmatrix} x \\ z \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} \Lambda\Lambda' + \Psi & \Lambda \\ \Lambda' & I \end{bmatrix} \right) .
$$

For two jointly distributed Gaussian (vector) variates,

$$\begin{bmatrix} x \\ z \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} a \\ b \end{bmatrix}, \begin{bmatrix} A & C \\ C' & D \end{bmatrix}\right) ,$$

the distribution of z given x is given by, see Zellner (1971),

$$z \,|\, x \sim \mathcal{N}\left(b + C'A^{-1}(x-a), \; D - C'A^{-1}C\right) .$$

Hence, in the FA model,

$$z \,|\, x \sim \mathcal{N}\left(Bx, \; I - B\Lambda\right) , \quad \text{where}$$

$$B = \Lambda'(\Lambda\Lambda' + \Psi)^{-1} = \left(\Psi^{-1} - \Psi^{-1}\Lambda\left(I + \Lambda'\Psi^{-1}\Lambda\right)^{-1}\Lambda'\Psi^{-1}\right)$$

C.5.1   EM Algorithm

In order to obtain the Maximum Likelihood (ML) estimator of the parameters, one can use the EM-Algorithm, see Rubin and Thayer (1982) and Russel (1998). The E-step for the FA model computes the expected first and second moments of the latent variables, for each observation, x.

$$E(z \,|\, x) = Bx , \quad \text{and}$$

$$E(zz' \,|\, x) = \text{Cov}(z \,|\, x) + E(z \,|\, x)E(z \,|\, x)' = I + B\Lambda + Bx \, x'B'$$

The M-step optimizes the parameters Λ and Ψ, of the expected log likelihood for the FA (completed data) model,

$$q(\Lambda, \Psi) = E\left(\log \prod_{j=1}^{n} f(x, z \,|\, \Lambda, \Psi)\right)$$

$$= E\left(\log \prod_{j=1}^{n} (2\pi)^{p/2} |\Psi|^{-1/2} \exp\left(-\frac{1}{2}\left(x^j - \Lambda z\right)' \Psi^{-1}\left(x^j - \Lambda z\right)\right)\right)$$

$$= c - \frac{n}{2} \log|\Psi| - \sum_{j=1}^{n} E\left(\frac{1}{2} x^{j'}\Psi^{-1}x^j - x^{j'}\Psi^{-1}\Lambda z + \frac{1}{2} z'\Lambda'\Psi^{-1}\Lambda z\right)$$

Using the results computed in the E-step, the last summation can be written as

$$\sum_{j=1}^{n}\left(\frac{1}{2} x^{j'}\Psi^{-1}x^j - x^{j'}\Psi^{-1}\Lambda E(z \,|\, x^j) + \frac{1}{2}\text{tr}\left(\Lambda'\Psi^{-1}\Lambda E(zz' \,|\, x^j)\right)\right)$$

The ML estimator, (Λ^*, Ψ^*), is a stationary point in Λ^*, therefore

$$\frac{\partial q}{\partial \Lambda} = -\sum_{j=1}^{n} \Psi^{-1}x^j E(z \,|\, x^j)' + \sum_{j=1}^{n} \Psi^{-1}\Lambda E(zz' \,|\, x^j) = 0 , \quad \text{hence}$$

$$\Lambda^* = \left(\sum_{j=1}^{n} E(zz' \,|\, x^j)'\right)^{-1} \sum_{j=1}^{n} x^j E(z \,|\, x^j)'$$

and also a stationary point in Ψ^*, or in its inverse, therefore, substituting the stationary value of Λ^* computed in the last equation,

$$\frac{\partial q}{\partial \Psi^{-1}} = \frac{n}{2}\Psi - \sum_{j=1}^{n}\left(\frac{1}{2}x^j x^{j\prime} - \Lambda^* E(z\,|\,x^j)x^{j\prime} + \frac{1}{2}\Lambda^* E(zz'\,|\,x^j)\Lambda^{*\prime}\right) = 0$$

Solving for Ψ, and using the diagonality constraint,

$$\Psi^* = \frac{1}{n}\mathrm{diag}^2\left(\sum_{j=1}^{n} x^j x^{j\prime} - \Lambda^* \sum_{j=1}^{n} E(z\,|\,x^j)x^{j\prime}\right)$$

The equation for Λ^*, in the M-step of the EM algorithm for FA, formally resembles the equation giving the LS estimation in a Linear Regression model, $\beta' = y'X(X'X)^{-1}$. This is why, in the FA literature, the matrix Λ^* is sometimes interpreted as "the linear regression coefficients of the z's on the x's".

C.5.2 Orthogonal and Oblique Rotations

Given a FA model and a non-singular coordinate transform, T, it is possible to obtain transformed factors together with transformed loadings giving an equivalent FA model. Both, a *direct*, and an *inverse*, form of the factor loadings transform are common in the literature.

In the direct form,
$$\widetilde{z} = T^{-1}z \text{ and } \widetilde{\Lambda} = \Lambda T,$$

hence, in the new model,

$$x = \Lambda z + u = \Lambda T T^{-1}z + u = \widetilde{\Lambda}\widetilde{z} + u \text{ and}$$

$$\mathrm{Cov}(x) = \widetilde{\Lambda}\widetilde{\Lambda}' + \Psi = \Lambda T(T^{-1}IT^{-t})T'\Lambda' + \Psi = \Lambda\Lambda' + \Psi .$$

In the inverse form,
$$\widetilde{z} = T'z \text{ and } \widetilde{\Lambda} = \Lambda T^{-t},$$

hence, in the new model,

$$x = \Lambda z + u = \Lambda T^{-t}T'z + u = \widetilde{\Lambda}\widetilde{z} + u \text{ and}$$

$$\mathrm{Cov}(x) = \widetilde{\Lambda}\widetilde{\Lambda}' + \Psi = \Lambda T^{-t}(T'IT)T^{-1}\Lambda' + \Psi = \Lambda\Lambda' + \Psi .$$

This shows that the FA model is only determined by the k dimensional subspace of $\mathcal{R}^p$ spanned by the factors. Any change of coordinates in this (sub) space, given by T, leads to an equivalent model.

An operator T is an *orthogonal rotation* iff $T'T = I$. Hence, orthogonal transformed factors are still normalized and uncorrelated.

An operator T is an *oblique rotation* (in the inverse form) iff $\mathrm{diag}^2(T'T) = I$. Hence, oblique transformed factors are still normalized, but correlated.

We want to chose either an orthogonal or an oblique rotation, T, so to minimize a complexity criterion function of $\widetilde{\Lambda}$. Before discussing appropriate criteria and how to use them, we examine some technical details concerning matrix norms and projections in the following subsection.

C.5.3   Frobenius Norm and Projections

The matrix Frobenius product and the matrix Frobenius norm are defined as follows:

$$\langle\, A \mid B \,\rangle_F = \mathrm{tr}(A'B) = \mathbf{1}'\,(A \odot B)\,\mathbf{1}\;,$$

$$||A||_F^2 = \langle\, A \mid A \,\rangle_F = \sum\nolimits_j \left|\left|A^j\right|\right|_2^2 = \sum\nolimits_i ||A_i||_2^2\;.$$

Lemma 1: The projection, T, with respect to the Frobenius norm, into the algebraic sub-manifold of the oblique rotation matrices

of a square matrix, A, is given as follows,

$$T = A\,\mathrm{diag}^2(A'A)^{1/2}\;.$$

A matrix T represents an *oblique rotation* iff it has normalized columns, that is, iff $\mathrm{diag}(T'T) = \mathbf{1}$. We want to minimize

$$||A - T||_F^2 = \sum\nolimits_j \left|\left|A^j - T^j\right|\right|_2^2$$

But, in the 2-norm, the normal vector T^j that is closest to the A^j is the one that has the same direction of vector A^j, that is,

$$T^j = \frac{1}{||A^j||_2}A^j = \frac{1}{(A^{j\prime}A^j)^{1/2}}A^j\;,$$

hence, the lemma.

Lemma 2: The projection, Q, with respect to the Frobenius norm, into the algebraic sub-manifold of the orthogonal rotation matrices of a square matrix, A, is given by its SVD factorization, as follows,

$$Q = UV'\;\;\text{where}\;\;U'(A)V = \mathrm{diag}(s)\;.$$

In order to prove the second lemma, we will consider the following problem. The *orthogonal Procrustes problem* seeks the orthogonal rotation, $Q \mid Q'Q = I$, that minimizes

the Frobenius norm of the difference between a given matrix A, $m \times p$, and the rotation of a second matrix, B, Formally, the problem is stated as

$$\min_{Q \,|\, Q'Q=I} ||A - BQ||_F^2$$

The norm function being minimized can be restated as

$$||A - BQ||_F^2 = \text{tr}(A'A) + \text{tr}(B'B) - 2\text{tr}(Q'B'A)$$

Hence the problem asks for the maximum of the last term. Let Z be an orthogonal matrix defined by Q and the SVD factorization of $B'A$ as follows,

$$U'(B'A)V = S = \text{diag}(s) \,, \quad Z = V'Q'U \,.$$

We have,
$$\text{tr}(Q'B'A) = \text{tr}(Q'USV') = \text{tr}(ZS) = s'\text{diag}(Z) \le s'\mathbf{1} \,.$$

But the last inequality is tight if $Z = I$, hence the optimal solution for the orthogonal Procrustes problem is

$$Q = UV' \quad \text{where} \quad U'(B'A)V = \text{diag}(s) \,.$$

In order to prove lemma 2, just consider the case $B = I$.

C.5.4   Sparsity Optimization

In the FA literature, minimizing the complexity of the factor loadings, $\widetilde{\Lambda}$, is accomplished by maximizing a measure of its sparsity, $f(\widetilde{\Lambda})$.

A natural sparsity measure in engineering applications is the Minimum Entropy measure. This measure and its (matrix) derivative are given by

$$f_{me}(\Lambda) = - \left\langle \Lambda 2 \,|\, \log(\Lambda 2) \right\rangle_F \,, \quad (\Lambda 2)_i^j = \left(\Lambda_i^j \right)^2 \,.$$

$$\frac{df_{me}(\Lambda)}{d\Lambda} = -\Lambda \odot \log(\Lambda 2) - \Lambda \,.$$

Several variations of the entropy sparsity measure are used in the literature, see Bernaards and Jennrich (2005).

Hoyer (2004) proposes the following sparsity measure for a vector $x \in \mathcal{R}_+^k$, based on the difference of two p-norms, namely $p = 1$ and $p = 2$,

$$f_{ho}(x) = \frac{1}{\sqrt{k} - 1} \left(\sqrt{k} - \frac{||x||_1}{||x||_2} \right) \,.$$

From Cauchy-Schwartz inequality, we have the bounds,

$$\frac{1}{\sqrt{n}}\,||x||_1 \leq ||x||_2 \leq ||x||_1 \;\;,\;\; \text{hence } 0 \leq f_{ho}(x) \leq 1 \;.$$

Similar interpretations can be given to the Carroll's Oblimin, on the parameter γ, and Crawford-Ferguson, on the parameter κ, families of sparsity measures. These measures, for Λ $p \times k$, and its (matrix) derivative are given by,

$$f_\gamma(\Lambda) = \frac{1}{4}\,\langle\,\Lambda2\,|\,B(\gamma)\,\rangle_F \;\;,\;\; \text{where}$$

$$B(\gamma) = (I - \gamma C)\Lambda2\,N \;\;,$$

$$(\Lambda2)_i^j = \left(\Lambda_i^j\right)^2 \;\;,\;\; C_i^j = \frac{1}{p} \;,\;\; N_i^j = 1 - \delta_i^j \;,\;\; \delta_i^j = \mathcal{I}(i = j)\;.$$

$$\frac{df_\gamma(\Lambda)}{d\Lambda} = \Lambda \odot B(\gamma)\;.$$

$$f_\kappa(\Lambda) = \frac{1}{4}\,\langle\,\Lambda2\,|\,B(\kappa)\,\rangle_F \;\;,\;\; \text{where}$$

$$B(\kappa) = (1 - \kappa)\Lambda2\,N + \kappa M\,\Lambda2 \;\;,$$

$$(\Lambda2)_i^j = \left(\Lambda_i^j\right)^2 \;\;,\;\; M_i^j = 1 - \delta_i^j \;, p \times p \;,\;\; N_i^j = 1 - \delta_i^j \;, k \times k\;.$$

$$\frac{df_\kappa(\Lambda)}{d\Lambda} = \Lambda \odot B(\kappa)\;.$$

These parametric families include many sparsity measures, or simplicity criteria, traditionally used in psychometric studies, for example, setting γ to 0, 1/2, or 1, we have the Quartmin, Biquartmin or Covarimin criterium, also, setting κ to 0, $1/p$, $k/(2p)$ or $(k-1)/(p+k-2)$, we have the Quartimax, Varimax, Equamax or Parsimax criterion.

In order to search for an optimal transformation, T^*, we need to express the sparsity function and its matrix derivative as functions of T. In the direct form,

$$\frac{df(\widetilde{\Lambda})}{dT} = \frac{df(\Lambda T)}{dT} = -\left(\Lambda'\frac{df(\Lambda)}{d\Lambda}\right)'\;.$$

In de inverse form,

$$\frac{df(\widetilde{\Lambda})}{dT} = \frac{df(\Lambda T^{-t})}{dT} = -\left(\Lambda'\frac{df(\Lambda)}{d\Lambda}T^{-1}\right)'\;.$$

This expressions, together with the projectors obtained in the last section, can be used in standard gradient projection optimization algorithms, like the Generalized Reduced Gradient (GRG) or other standard primal optimization algorithms, see Bernaards and Jennrich (2005), Jennrich (2002), Luenberger (1984), Minoux and Vajda (1986), Shah et al. (1964), and Stern et al. (2006).

The projection operation for oblique rotations only requires inexpensive matrix operations, like a matrix inversion, performed numerically as a LU or QR factorization. The projection operation for orthogonal rotations, on the other hand, requires a SVD factorization, an operation that requires much more computational work. Therefore, a constraint free representation of an orthogonal matrix can be very useful in designing optimization algorithms, see Browne (1974, 2001). The Cayley transform establishes one-to-one correspondence between skew-symmetric operators, K, and the orthogonal operators, Q, that do not have -1 as a characteristic value, see Gantmacher (1959, I, 288-289). Although extreme reversal operators, like a coordinate reflection or permutation can not be represented in this form, there is a Cayley representation for any local, that is, not too far from the identity, orthogonal operator.

$$J = K + I \ , \quad K_i^j = -K_j^i \ .$$

$$K = (I - Q)(I + Q)^{-1} = 2(I + Q)^{-1} - I \ ,$$

$$Q = (I - K)(I + K)^{-1} = 2J^{-1} - I \ .$$

The spasity measure derivatives of the direct orthogonal rotation of the factor loadings, using the Cayley representation, are given by,

$$f(\widetilde{\Lambda}) = f(\Lambda T) \ , \quad T = J^{-1} - I$$

$$\frac{\partial f(\widetilde{\Lambda})}{\partial J_i^j} = \mathrm{tr}\left(\frac{\partial f(\widetilde{\Lambda})}{\partial T'}\frac{\partial T}{\partial J_i^j}\right) = -2\mathrm{tr}\left(\frac{\partial f(\widetilde{\Lambda})'}{\partial T}J^{-1}\frac{\partial J}{\partial J_i^j}J^{-1}\right) =$$

$$2(Y_i^j - Y_j^i) \ , \quad \text{where} \ \ Y = J^{-1}\frac{\partial f(\widetilde{\Lambda})'}{\partial T}J^{-1} \ .$$

C.6 Mixture Models

The matrix notation used in this section is defined in section F.1. In this section, h, i are indices in the range $1{:}d$, k is in $1{:}m$, and j is in $1{:}n$.

In a d-dimensional multivariate finite mixture model with m components (or classes), and sample size n, any given sample x^j is of class k with probability w_k; the weights, w_k, give the probability that a new observation is of class k. A sample j of class $k = c(j)$ is distributed with density $f(x^j \,|\, \psi_k)$.

The classifications z_k^j are boolean variables indicating whether or not x^j is of class k, i.e. $z_k^j = 1$ iff $c(j) = k$. Z is not observed, being therefore named latent variable or missing data. Conditioning on the missing data, we get:

$$\begin{aligned} f(x^j \,|\, \theta) &= \sum_{k=1}^m f(x^j \,|\, \theta, z_k^j) f(z_k^j \,|\, \theta) &= \sum_{k=1}^m w_k f(x^j \,|\, \psi_k) \\ f(X \,|\, \theta) &= \prod_{j=1}^n f(x^j \,|\, \theta) &= \prod_{j=1}^n \sum_{k=1}^m w_k f(x^j \,|\, \psi_k) \end{aligned}$$

Given the mixture parameters, θ, and the observed data, X, the conditional classification probabilities, $P = f(Z \mid X, \theta)$, are:

$$p_k^j \;\; = \;\; f(z_k^j \mid x^j, \theta) \;\; = \;\; \frac{f(z_k^j, x^j \mid \theta)}{f(x^j \mid \theta)} \;\; = \;\; \frac{w_k f(x^j \mid \psi_k)}{\sum_{k=1}^m w_k f(x^j \mid \psi_k)}$$

We use y_k for the number of samples of class k, i.e. $y_k = \sum_j z_k^j$, or $y = Z\mathbf{1}$. The likelihood for the "completed" data, X, Z, is:

$$f(X, Z \mid \theta) \;\; = \;\; \prod_{j=1}^n f(x^j \mid \psi_{c(j)}) f(z_k^j \mid \theta) \;\; = \;\; \prod_{k=1}^m \Big(w_k{}^{y_k} \prod_{j \mid c(j)=k} f(x^j \mid \psi_k) \Big)$$

We will see in the following sections that considering the missing data Z, and the conditional classification probabilities P, is the key for successfully solving the numerical integration and optimization steps of the FBST. In this article we will focus on Gaussian finite mixture models, where $f(x^j \mid \psi_k) = N(x^j \mid b^k, R\{k\})$, a normal density with mean b^k and variance matrix $V\{k\}$, or precision $R\{k\} = (V\{k\})^{-1}$. Next we specialize the theory of general mixture models to the Dirichlet-Normal-Wishart case.

C.6.1 Dirichlet-Normal-Wishart Mixtures

Consider the random matrix X_i^j, i in $1\!:\!d$, j in $1\!:\!n$, $n > d$, where each column contains a sample element from a d-multivariate normal distribution with parameters b (mean) and V (covariance), or $R = V^{-1}$ (precision). Let u and S denote the statistics:

$$u = (1/n) \sum_{j=1}^n x^j = (1/n)\, X\mathbf{1} \;\; , \quad S = \sum_{j=1}^n (x^j - b) \otimes (x^j - b)' = (X - b)(X - b)'$$

The random vector u has normal distribution with mean b and precision nR. The random matrix S has Wishart distribution with n degrees of freedom and precision matrix R. The Normal, Wishart and Normal-Wishart pdfs have expressions:

$$N(u \mid n, b, R) = \left(\tfrac{n}{2\pi}\right)^{d/2} |R|^{1/2} \exp\big(-(n/2)(u - b)' R(u - b) \big)$$

$$W(S \mid e, R) = c^{-1} |S|^{(e-d-1)/2} \exp\big(-(1/2)\mathrm{tr}(S\,R) \big)$$

with normalization constant $\;c = |R|^{-e/2}\, 2^{ed/2}\, \pi^{d(d-1)/4} \prod_{i=1}^d \Gamma((e - i + 1)/2)\;$.

Now consider the matrix X as above, with unknown mean b and unknown precision matrix R, and the statistic

$$S = \sum_{j=1}^n (x^j - u) \otimes (x^j - u)' = (X - u)(X - u)'$$

The conjugate family of priors for multivariate normal distributions is the Normal-Wishart, see DeGroot (1970). Take as prior distribution for the precision matrix R the

wishart distribution with $\dot{e} > d - 1$ degrees of freedom and precision matrix $\dot{S}$ and, given R, take as prior for b a multivariate normal with mean $\dot{u}$ and precision $\dot{n}R$, i.e. let us take the Normal-Wishart prior $NW(b, R \,|\, \dot{n}, \dot{e}, \dot{u}, \dot{S})$. Then, the posterior distribution for R is a Wishart distribution with $\ddot{e}$ degrees of freedom and precision $\ddot{S}$, and the posterior for b, given R, is k-Normal with mean $\ddot{u}$ and precision $\ddot{n}R$, i.e., we have the Normal-Wishart posterior:

$$
\begin{aligned}
NW(b, R \,|\, \ddot{n}, \ddot{e}, \ddot{u}, \ddot{S}) &= W(R \,|\, \ddot{e}, \ddot{S}) \, N(b \,|\, \ddot{n}, \ddot{u}, R) \\
\ddot{n} &= \dot{n} + n \;\; , \;\; \ddot{e} = \dot{e} + n \;\; , \;\; \ddot{u} = (nu + \dot{n}\dot{u})/\ddot{n} \\
\ddot{S} &= S + \dot{S} + (n\dot{n}/\ddot{n})(u - \dot{u}) \otimes (u - \dot{u})'
\end{aligned}
$$

All covariance and precision matrices are supposed to be positive definite, and proper priors have $\dot{e} \geq d$, and $\dot{n} \geq 1$. Non-informative Normal-Wishart improper priors are given by $\dot{n} = 0$, $\dot{u} = 0$, $\dot{e} = 0$, $\dot{S} = 0$, i.e. we take a Wishart with 0 degrees of freedom as prior for R, and a constant prior for b, see DeGroot (1970). Then, the posterior for R is a Wishart with n degrees of freedom and precision S, and the posterior for b, given R, is d-Normal with mean u and precision nR.

The conjugate prior for a multinomial distribution is a Dirichlet distribution:

$$
\begin{aligned}
M(y \,|\, n, w) &= \left(n!/y_1! \ldots y_m!\right) w_1{}^{y_1} \ldots w_m{}^{y_m} \\
D(w \,|\, y) &= \left(\Gamma(y_1 + \ldots + y_k)/\Gamma(y_1) \ldots \Gamma(y_k)\right) \prod_{k=1}^{m} w_k{}^{y_k - 1}
\end{aligned}
$$

with $w > \mathbf{0}$ and $w\mathbf{1} = 1$. Prior information given by $\dot{y}$, and observation y, result in the posterior parameter $\ddot{y} = \dot{y} + y$. A non-informative prior is given by $\dot{y} = \mathbf{1}$.

Finally, we can write the posterior and completed posterior for the model as:

$$
f(\theta \,|\, X, \dot{\theta}) = f(X \,|\, \theta) f(\theta \,|\, \dot{\theta})
$$

$$
f(X \,|\, \theta) = \prod_{j=1}^{n} \sum_{k=1}^{m} p_k^j w_k N(x^j \,|\, b^k, R\{k\})
$$

$$
f(\theta \,|\, \dot{\theta}) = D(w \,|\, \dot{y}) \prod_{k=1}^{m} NW(b^k, R\{k\} \,|\, \dot{n}_k, \dot{e}_k, \dot{u}^k, \dot{S}\{k\})
$$

$$
p_k^j = w_k N(x^j \,|\, b^k, R\{k\}) \,/\, \sum_{k=1}^{m} w_k N(x^j \,|\, b^k, R\{k\})
$$

$$
f(\theta \,|\, X, Z, \dot{\theta}) = f(\theta \,|\, X, Z) f(\theta \,|\, \dot{\theta}) = D(w \,|\, \ddot{y}) \prod_{k=1}^{m} NW(b^k, R\{k\} \,|\, \ddot{n}_k, \ddot{e}_k, \ddot{u}^k, \ddot{S}\{k\})
$$

$$
y = Z\mathbf{1} \;\; , \;\; \ddot{y} = \dot{y} + y \;\; , \;\; \ddot{n} = \dot{n} + y \;\; , \;\; \ddot{e} = \dot{e} + y
$$

$$
u^k = (1/y_k) \sum_{j=1}^{n} z_k^j x^j \;\; , \;\; S\{k\} = \sum_{j=1}^{n} z_k^j (x^j - u^k) \otimes (x^j - u^k)'
$$

$$
\ddot{u}^k = (1/\ddot{y}_k)(\dot{n}_k \dot{u}^k + y_k u^k) \;\; , \;\; \ddot{S}\{k\} = S\{k\} + \dot{S}\{k\} + (\dot{n}_k y_k / \ddot{n}_k)(u^k - \dot{u}^k) \otimes (u^k - \dot{u}^k)'
$$

C.6.2   Gibbs Sampling and Integration

In order to integrate a function over the posterior measure, we use an ergodic Markov Chain. The form of the Chain below is known as Gibbs sampling, and its use for numerical integration is known as Markov Chain Monte Carlo, or MCMC.

Given θ, we can compute P. Given P, $f(z^j \mid p^j)$ is a simple multinomial distribution. Given the latent variables, Z, we have simple conditional posterior density expressions for the mixture parameters:

$$f(w \mid Z, \dot{y}) = D(w \mid \ddot{y}) \quad , \quad f(R\{k\} \mid X, Z, \dot{e}_k, \dot{S}\{k\}) = W(R \mid \ddot{e}_k, \ddot{S}\{k\})$$

$$f(b^k \mid X, Z, R\{k\}, \dot{n}_k, \dot{u}^k) = N(b \mid \ddot{n}_k, \ddot{u}^k, R\{k\})$$

Gibbs sampling is nothing but the MCMC generated by cyclically updating variables Z, θ, and P, by drawing θ and Z from the above distributions, see Gilks aet al. (1996) and Häggström (2002). A uniform generator is all what is needed to the multinomial variate. A Dirichlet variate w can be drawn using a gamma generator with shape and scale parameters α and β, $G(\alpha, \beta)$, see Gentle (1998). Johnson (1987) describes a simple procedure to generate the Cholesky factor of a Wishart variate $W = U'U$ with n degrees of freedom, from the Cholesky factorization of the covariance $V = R^{-1} = C'C$, and a chi-square generator: a) $g_k = G(y_k, 1)$; b) $w_k = g_k \,/\, \sum_{k=1}^m g_k$; c) for $i < j$, $B_{i,j} = N(0, 1)$; d) $B_{i,i} = \sqrt{\chi^2(n - i + 1)}$; and e) $U = BC$. All subsequent matrix computations proceed directly from the Cholesky factors, see Jones (1985).

Label Switching and Forbidden States

Given a mixture model, we obtain an equivalent model renumbering the components $1\!:\!m$ by a permutation $\sigma([1\!:\!m])$. This symmetry must be broken in order to have an identifiable model, see Stephens (1997). Let us assume there is an order criterion that can be used when numbering the components. If the components are not in the correct order, Label Switching is the operation of finding permutation $\sigma([1\!:\!m])$ and renumbering the components, so that the order criterion is satisfied. If we want to look consistently at the classifications produced during a MCMC run, we must enforce a label switching to break all non-identifiability symmetries. For example, in the Dirichlet-Normal-Mixture model, we could choose to order the components (switch labels) according to the the rank given by: 1) A given linear combination of the vector means, $c' * b^k$; 2) The variance determinant $|V\{k\}|$. The choice of a good label switching criterion should consider not only the model structure and the data, but also the semantics and interpretation of the model.

The semantics and interpretation of the model may also dictate that some states, like certain configurations of the latent variables Z, are either meaningless or invalid, and

shall not be considered as possible solutions. The MCMC can be adapted to deal with forbidden states by implementing rejection rules, that prevent the chain from entering the forbidden regions of the complete and/or incomplete state space, see Bennett (1976) and Meng (1996).

C.6.3   EM Algorithm for ML and MAP Estimation

The EM algorithm optimizes the log-posterior function $fl(X \mid \theta) + fl(\theta \mid \dot\theta)$, see Dempster (1977), Ormoneit (1995) and Russel (1988). The EM is derived from the conditional log-likelihood, and the Jensen inequality: If $w, y > \mathbf{0}, w'\mathbf{1} = 1$ then $\log w'y \geq w' \log y$. Let θ and $\tilde\theta$ be our current and next estimate of the MAP (Maximum a Posteriori), and $p_k^j = f(z_k^j \mid x^j, \theta)$ the conditional classification probabilities. At each iteration, the log-posterior improvement is:

$$\delta(\tilde\theta, \theta \mid X, \dot\theta) \;=\; fl(\tilde\theta \mid X, \dot\theta) - fl(\theta \mid X, \dot\theta) \;=\; \delta(\tilde\theta, \theta \mid X) + \delta(\tilde\theta, \theta \mid \dot\theta)$$

$$\delta(\tilde\theta, \theta \mid \dot\theta) \;=\; fl(\tilde\theta \mid \dot\theta) - fl(\theta \mid \dot\theta)$$

$$\delta(\tilde\theta, \theta \mid X) \;=\; fl(X \mid \tilde\theta) - fl(X \mid \theta) \;=\; \sum_j \delta(\tilde\theta, \theta \mid x^j)$$

$$\delta(\tilde\theta, \theta \mid x^j) \;=\; fl(x^j \mid \tilde\theta) - fl(x^j \mid \theta) \;=\; \log \sum_k \tilde w_k f(x^j \mid \tilde\psi_k) \; - fl(x^j \mid \theta) \;=$$

$$=\; \log \sum_k \frac{p_k^j}{p_k^j} \frac{\tilde w_k f(x^j \mid \tilde\psi_k)}{f(x^j \mid \theta)} \;\geq\; \Delta(\tilde\theta, \theta \mid x^j) \;=\; \sum_k p_k^j \log \frac{\tilde w_k f(x^j \mid \tilde\psi_k)}{p_k^j f(x^j \mid \theta)}$$

Hence, $\Delta(\tilde\theta, \theta \mid X, \dot\theta) = \Delta(\tilde\theta, \theta \mid X) + \delta(\tilde\theta, \theta \mid \dot\theta)$, is a lower bound to $\delta(\tilde\theta, \theta \mid X, \dot\theta)$. Also $\Delta(\theta, \theta \mid X, \dot\theta) = \delta(\theta, \theta \mid X, \dot\theta) = 0$. So, under mild differentiability conditions, both surfaces are tangent, assuring convergence of EM to the nearest local maximum. But maximizing $\Delta(\tilde\theta, \theta \mid X, \dot\theta)$ over $\tilde\theta$ is the same as maximizing

$$Q(\tilde\theta, \theta) \;=\; \sum_{k,j} p_k^j \log\left(\tilde w_k f(x^j \mid \tilde\psi_k) \right) + fl(\tilde\theta \mid \dot\theta)$$

and each iteration of the EM algorithm breaks down in two steps:

E-step: Compute $P = E(Z \mid X, \theta)$.

M-step: Optimize $Q(\tilde\theta, \theta)$, given P.

For the Gaussian mixture model, with a Dirichlet-Normal-Wishart prior,

$$Q(\tilde\theta, \theta) \;=\; \sum_{k=1}^m \sum_{j=1}^n p_k^j \left(\log \tilde w_k + \log N(x^j \mid \tilde b^k, \tilde R\{k\}) \right) + fl(\tilde\theta \mid \dot\theta)$$

$$fl(\tilde\theta \mid \dot\theta) \;=\; \log D(\tilde w \mid \dot y) + \sum_{k=1}^m \log NW(\tilde b^k, \tilde R\{k\} \mid \dot n_k, \dot e_k, \dot u^k, \dot S\{k\})$$

Lagrange optimality conditions give a simple analytical solutions for the M-step:

$$y = P\mathbf{1} \;\;,\;\; \tilde w_k = (y_k + \dot y_k - 1) \left/ \left(n - m + \sum_{k=1}^m \dot y_k \right) \right.$$

$$u^k = \frac{1}{y_k} \sum_{j=1}^{n} p_k^j x^j \quad , \quad S\{k\} = \sum_{j=1}^{n} p_k^j (x^j - \tilde{b}^k) \otimes (x^j - \tilde{b}^k)'$$

$$\tilde{b}^k = \frac{\dot{n}_k \dot{u}^k + y_k u^k}{\dot{n}_k + y_k} \quad , \quad \tilde{V}^k = \frac{S\{k\} + \dot{n}_k (\tilde{b}^k - \dot{u}^k) \otimes (\tilde{b}^k - \dot{u}^k)' + \dot{S}\{k\}}{y_k + \dot{e}_k - d}$$

Global Optimization

In more general (non-Gaussian) mixture models, if an analytical solution for the M-step is not available, a robust local optimization algorithm can be used, for example Martinez (2000). The EM is only a local optimizer, but the MCMC provides plenty of good starting points, so we have the basic elements for a global optimizer. To avoid using many starting points going to a same local maximum, we can filter the (ranked by the posteriori) top portion of the MCMC output using a clustering algorithm, and select a starting point from each cluster. For better efficiency, or more complex problems, the Stochastic EM or SEM algorithm can be used to provide starting points near each important local maximum, see Celeux (1995), Pflug (1996) and Spall (2003).

C.6.4 Experimental Tests and Final Remarks

The test case used in this study is given by a sample X assumed to follow a mixture of bivariate normal distributions with unknown parameters, including the number of components. X is the *Iris virginica* data set, with sepal and petal length of 50 specimens (1 discarded outlier). The botanical problem consists of determining whether or not there are two distinct subspecies in the population, see Anderson (1935), Fisher (1936) and McLachlan (2000). Figure 1 presents the dataset and posterior density level curves for the parameters, θ^* and $\widehat{\theta}$, optimized for the 1 and 2 component models.
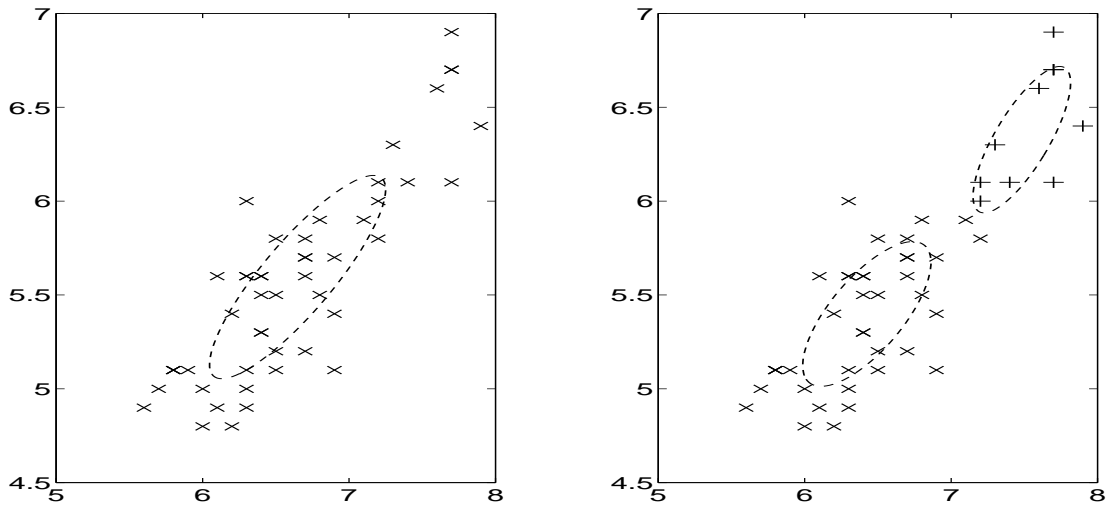
Figure1: Iris virginica data and models with one (left) and two (right) components

In the FBST formulation of the problem, the 2 components is the base model, and the hypothesis to be tested is the constraint of having only 1 component. When implementing the FBST one has to be careful with trapping states on the MCMC. These typically are states where one component has a small number of sample points, that become (nearly) collinear, resulting in a singular posterior. This problem is particularly serious with the Iris dataset because of the small precision, only 2 significant digits, of the measurements. A standard way to avoid this inconvenience is to use flat or minimally informative priors, instead of non-informative priors, see Robert (1996).

We used as flat prior parameters: $\dot{y} = \mathbf{1}$, $\dot{n} = 1$, $\dot{u} = u$, $\dot{e} = 3$, $\dot{S} = (1/n)S$. Robert (1996) uses, with similar effects, $\dot{e} = 6$, $\dot{S} = (1.5/n)S$.

The FBST selects the 2 component model, rejecting H, if the evidence against the hypothesis is above a given threshold, $\mathrm{ev}(H) > \tau$, and selects the 1 component model, accepting H, otherwise. The threshold τ is chosen by empirical power analysis, see Stern and Zacks (2002) and Lauretto et al. (2003). Let θ^* and $\widehat{\theta}$ represent the constrained (1 component) and unconstrained (2 component) maximum a posteriori (MAP) parameters optimized to the Iris dataset. Next, generate two collections of t simulated datasets of size n, the first collection at θ^*, and the second at $\widehat{\theta}$. $\alpha(\tau)$ and $\beta(\tau)$, the empirical type 1 and type 2 statistical errors, are the rejection rate in the first collection and the acceptance rate in the second collection. A small, $t = 500$, calibration run sets the threshold τ so to minimize the total error, $(\alpha(\tau) + \beta(\tau))/2$. Other methods like sensitivity analysis, see Stern (2004a,b), and loss functions, see Madruga (2001), could also be used.

Biernacki and Govaert (1998) studied similar mixture problems and compared several selection criteria, pointing as the best overall performers: AIC - Akaike Information Criterion, AIC3 - Bozdogan's modified AIC, and BIC - Schwartz' Bayesian Information Criterion. These are regularization criteria, weighting the model fit against the number of parameters, see Pereira and Stern (2001). If λ is the model log-likelihood, κ its number of parameters, and n the sample size, then,

$$AIC = -2\lambda + 2\kappa \ , \quad AIC3 = -2\lambda + 3\kappa \ \text{and} \ \ BIC = -2\lambda + \kappa \log(n) \ .$$

Figure 2 show α, β, and the total error $(\alpha + \beta)/2$. The FBST outperforms all the regularization criteria. For small samples, BIC is very biased, always selecting the 1 component model. AIC is the second best criterion, caching up with the FBST for sample sizes larger than $n = 150$.
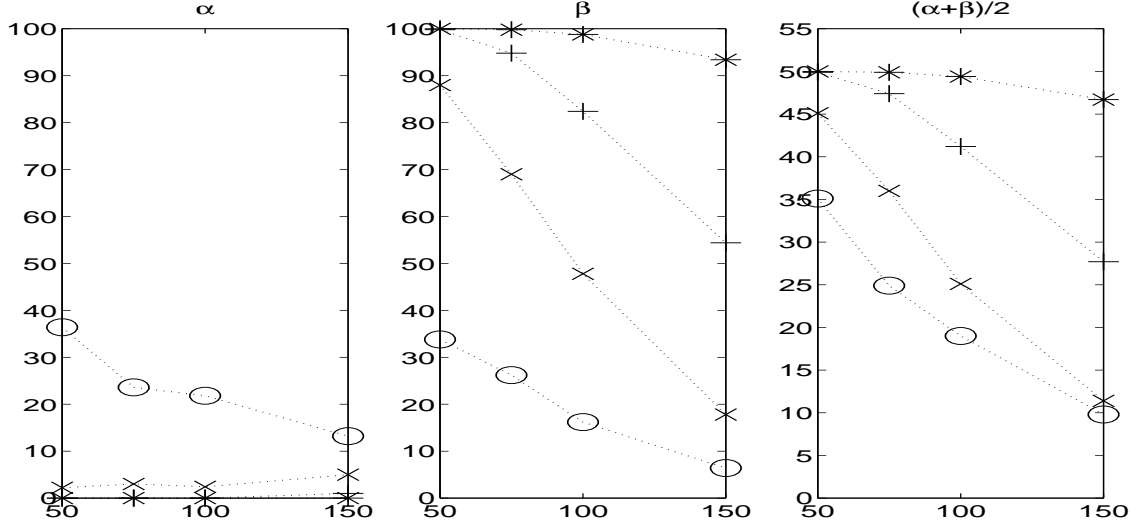
Figure 2: Criteria O= FBST, X= AIC, += AIC3, *= BIC,
Type 1, 2 and total error rates for different sample sizes

Finally, let us point out a related topic for further research: The problem of discriminating between models consists of determining which of m alternative models, $f_k(x, \psi_k)$, more adequately fits or describes a given dataset. In general the parameters ψ_k have distinct dimensions, and the models f_k have distinct (unrelated) functional forms. In this case it is usual to call them "separate" models (or hypotheses). Atkinson (1970), although in a very different theoretical framework, was the first to analyse this problem using a mixture formulation,

$$f(x \mid \theta) = \sum\nolimits_{k=1}^{m} w_k f_k(x, \psi_k) \ .$$

The general theory for mixture models presented in this article can be adapted to analyse the problem of discriminating between separate hypotheses. This is the subject of the authors' ongoing research with Carlos Alberto de Bragança Pereira and Basílio de Bragança Pereira, to be presented in forthcoming articles.

C.7   REAL Classification Trees

This section presents an overview of REAL, The Real Attribute Learning Algorithm for automatic construction of classification trees. The REAL project started as an application to be used at the Brazilian BOVESPA and BM&F financial markets, trying to provide a good algorithm for predicting the adequacy of operation strategies. In this context, the

success or failure of a given operation strategy corresponds to different classes, and the attributes are real-valued technical indicators. The users demands for a decision support tool also explain several of the algorithm's unique features.

The classification problems are stated as an $n \times (m + 1)$ matrix A. Each row, $A(i, :)$, represents a different example, and each column, $A(:, j)$, a different attribute. The first m columns in each row are real-valued attributes, and the last column , $A(i, m + 1)$ is the example's class. Part of these samples, the training set, is used by the algorithm to generate a classification tree, which is then tested with the remaining examples. The error rate in the classification of the examples in the test set is a simple way of evaluating the classification tree.

A market operation strategy is a predefined set of rules determining an operator's actions in the market. The strategy shall have a predefined criterion for classifying a strategy application as success or failure.

As a simple example, let us define the strategy $buysell(t, d, l, u, c)$:

- At time t buy a given asset A, at its price $p(t)$.

- Sell A as soon as:

  1. $t' = t + d$, or
  2. $p(t') = p(t) * (1 + u/100)$, or
  3. $p(t') = p(t) * (1 - l/100)$.

- The strategy application is successful if $c \leq 100 * p(t')/(p(t) \leq u$

The parameters u, l, c and d can be interpreted as the desired and worst accepted returns (low and upper bound), the strategy application cost, and a time limit.

Tree Construction

Each main iteration of the REAL algorithm corresponds to the branching of a terminal node in the tree. The examples at that node are classified according to the value of a selected attribute, and new branches generated to each specific interval. The partition of a real-valued attribute's domain in adjacent non-overlapping (sub) intervals is the discretization process. Each main iteration of REAL includes:

1. The discretization of each attribute, and its evaluation by a loss function.

2. Selecting the best attribute, and branching the node accordingly.

3. Merging adjacent intervals that fail to reach a minimum conviction threshold.

C.7.1   Conviction, Loss and Discretization

Given a node of class c with n examples, k of which are misclassified and $(n-k)$ of which are correctly classified, we needed a single scalar parameter, cm, to measure the probability of misclassification and its confidence level. Such a simplified conviction (or trust) measure was a demand of REAL users operating at the stock market.

Let q be the misclassification probability for an example at a given node, let $p = (1-q)$ be the probability of correct classification, and assume we have a Bayesian distribution for q , namely

$$D(c) = Pr(q \leq c) = Pr(p \geq 1 - c)$$

We define the conviction measure: $100 * (1 - cm)\%$, where

$$cm = \min c \quad | \quad Pr(q \leq c) \geq 1 - g(c)$$

and $g(\ )$ is a monotonically increasing bijection of $[0, 1]$ onto itself. From our experience in the stock market application we learned to be extra cautious about making strong statements, so we make $g(\ )$ a convex function.

In this paper $D(c)$ is the posterior distribution for a sample taken from the Bernoulli distribution, with a uniform prior for q:

$$
\begin{aligned}
B(n, k, q) &= comb(n, k) * q^k * p^{n-k} \\
D(c, n, k) &= \int_{q=0}^{c} B(n, k, q) \quad / \quad \int_{q=0}^{1} B(n, k, q) \\
&= \mathrm{betainc}(c, k + 1, n - k + 1)
\end{aligned}
$$

Also in this paper, we focus our attention on

$$g(c) = g(c, r) = c^r, \quad r \geq 1.0$$

we call r the convexity parameter.

With these choices, the posterior is the easily computed incomplete beta function, and cm is the root of the monotonically decreasing function:

$$
\begin{aligned}
cm(n, k, r) &= c \quad | \quad f(c) = 0 \\
f(c) &= 1 - g(c) - D(c, n, k) \\
&= 1 - c^r - \mathrm{betainc}(c, k + 1, n - k + 1)
\end{aligned}
$$

Finally, we want a loss function for the discretizations, based on the conviction measure. In this paper we use the overall sum of each example classification conviction, that

is, the sum over all intervals of the interval's conviction measure times the number of examples in the interval.

$$loss = \sum_i n_i * cm_i$$

Given an attribute, the first step of the discretization procedure is to order the examples in the node by the attribute's value, and then to join together the neighboring examples of the same class. So, at the end of this first step, we have the best ordered discretization for the selected attribute with uniform class clusters.

In the subsequent steps, we join intervals together, in order to decrease the overall loss function of the discretization. The gain of joining J adjacent intervals, I_{h+1}, I_{h+2}, $\ldots I_{h+J}$, is the relative decrease in the loss function

$$gain(h, j) = \sum_j loss(n_j, k_j, r) \quad - loss(n, k, r)$$

where $n = \sum_j n_j$ and k counts the minorities' examples in the new cluster (at the second step $k_j = 0$, because we begin with uniform class clusters).

At each step we perform the cluster joining operation with maximum gain. The discretization procedure stops when there are no more joining operations with positive gain.

The next examples show some clusters that would be joined together at the first step of the discretization procedure. The notation $(n, k, m, r, \pm)$ means the we have two uniform clusters of the same class, of size n and m, separated by a uniform cluster of size k of a different class; r is the convexity parameter, and $+$ $(-)$ means we would (not) join the clusters together.

```
( 2,1, 2,2,+)
( 6,2, 7,2,-) ( 6,2, 8,2,+) ( 6,2,23,2,+) ( 6,2,24,2,-)
( 7,2, 6,2,-) ( 7,2, 7,2,+) ( 7,2,42,2,+) ( 7,2,43,2,-)
(23,3,23,2,-) (23,3,43,2,-) (23,3,44,2,+)
(11,3,13,3,-) (11,3,14,3,+) (11,3,39,3,+) (11,3,40,3,-)
(12,3,12,3,-) (12,3,13,3,+) (12,3,54,3,+) (12,3,55,3,-)
```

In these examples we see that it takes extreme clusters of a balanced and large enough size, n and m, to "absorb" the noise or impurity in the middle cluster of size k. A larger convexity parameter, r, implies a larger loss at small clusters, and therefore makes it easier for sparse impurities to be absorbed.

C.7.2   Branching and Merging

For each terminal node in the tree, we

1. perform the discretization procedure for each available attribute,

2. measure the loss function of the final discretization,

3. select the minimum loss attribute, and

4. branch the node according this attribute discretization.

If no attribute discretization decreases the loss function by a numerical precision threshold $\epsilon > 0$, no branching takes place.

A premature discretization by a parameter selected at a given level may preclude further improvement of the classification tree by the branching process. For this reason we establish a conviction threshold, ct, and after each branching step we merge all adjacent intervals that do not achieve $cm < ct$. To prevent an infinite loop, the loss function value assigned to the merged interval is sum of the losses of the merging intervals. At the final leaves, this merging is undone. The conviction threshold naturally stops the branching process, so there is no need for an external pruning procedure, like in most TDIDT algorithms.

In the straightforward implementation, REAL spends most of the execution time computing the function $cm(n, k, r)$. We can greatly accelerate the algorithm by using precomputed tables of $cm(n, k, r)$ values for small n, and precomputed tables of $cm(n, k, r)$ polynomial interpolation coefficients for larger n. To speed up the algorithm we can also restrict the search for join operations at the discretization step to small neighborhoods, i.e. to join only $3 \leq J \leq Jmax$ clusters: Doing so will expedite the algorithm without any noticeable consistent degradation.

For further details on the numerical implementation, benchmarks, and the specific market application, see Lauretto et al. (1998).

Appendix D

Deterministic Evolution and Optimization

This chapter presents some methods of deterministic optimization. Section 1 presents the fundamentals of Linear Programming (LP), its duality theory, and some variations of the Simplex algorithm. Section 2 presents some basic facts of constrained and unconstrained Non-Linear Programming (NLP), the Generalized Reduced Gradient (GRG) algorithm for constrained NLP problems, the ParTan method for unconstrained NLP problems, and some simple line search algorithms for uni-dimensional problems. Sections 1 and 2 also presents some results about these algorithms local and global convergence properties. Section 3 is a very short introduction to variational problems and the Euler-Lagrange equation.

The algorithms presented in sections 1 and 2 are within the class of *active set* or active constraint algorithms. The choice of concentrating on this class is motivated by some properties of active set algorithms, that makes them specially useful in the applications concerning the statistics, namely:

- Active set algorithms maintain viability throughout in the search path for the optimal solution. This is important if the objective function can only be computed at (nearly) feasible arguments, as it is often the case in statistics or simulation problems. This feature also makes active set algorithms relatively easy to expalain and implement.

- The general convergence theory of active set algorithms and the analysis of specific problems may offer a constructive proof of the existence or the verification of stability conditions for an equilibrium or fixed point, representing a systemic eigen-solution see, for example, Border (1989), Ingrao and Israel (1990) and Zangwill (1964).

- Active set algorithms are particularly efficient for small or medium size re-optimization problems, that is, for optimization problems where the initial solution or staring point for the optimization procedure is (nearly) feasible and already close to the optimal solution,

so that the optimization algorithm is only used to finetune the solution. In FBST applications, such good staring points can be obtained from an exploratory search performed by the Monte Carlo or Markov Chain Monte Carlo procedures used to numerically integrate the FBST e-value, $\text{ev}(H)$, or truth function $W(v)$, see appendices A and G.

D.1   Convex Sets and Polyedra

The matrix notation used in this book is defined at section F.1.

Convex Sets

A point $y(l)$ is a *convex combination* of m points of R^n, given by the columns of matrix X, $n \times m$, iff

$$\forall i ,\quad y(l)_i = \sum_{j=1}^{m} l_j * X_i^j ,\quad l_j \geq 0 \mid \sum_{j=1}^{m} l_j = 1 ,$$

or, equivalently, in matrix notation, iff

$$y(l) = \sum_{i=1}^{m} l_i * X^j ,\quad l_j \geq 0 \mid \sum_{j=1}^{m} l_j = 1 ,$$

or, in yet another equivalent form, replacing the summations by inner products,

$$y(l) = Xl ,\quad l \geq 0 \mid \mathbf{1}'l = 1 .$$

In particular, the point $y(\lambda)$ is a convex combination of two points, z e w, if

$$y(\lambda) = (1 - \lambda)z + \lambda w ,\quad \lambda \in [0,\ 1] .$$

Geometrically, these are the points in the line segment from z to w.

A set, $C \in R^n$, is *convex* iff it contains all convex combinations of any two of its points. A set, $C \in R^n$, is *bounded* iff the distance between any two of its points is bounded:

$$\exists \delta \mid \forall x1,\ x2 \in C ,\quad ||x1 - x2|| \leq \delta$$

Figure D.1 presents some sets exemplifying the definitions above.

An *extreme point* of a convex set C is a point $x \in C$ that can not be represented as a convex combination of two other points of C. The *profile* of a convex set C, $\text{ext}(C)$, is the set of its extreme points. The *Convex hull* and the *closed convex hull* of a set C, $\text{ch}(C)$ and $\text{cch}(C)$, are the intersection of all convex sets, and closed convex sets, containing C.

Theorem: A compact (closed and bounded) convex set is equal to the closed convex hull of its profile, that is, $C = \text{cch}(\text{ext}(C))$.
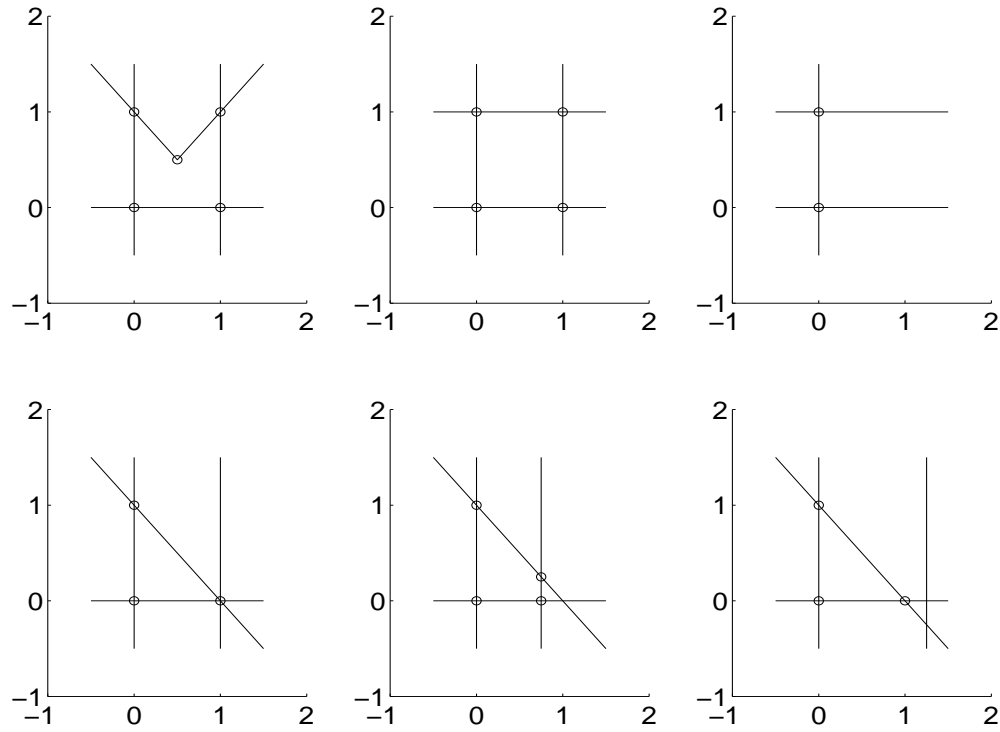
Figure D.1: (a) non-convex set, (b,c) bounded and unbounded polyedron, (d-f) degenerate vertex perturbed to a single or two nondegenerate ones.

The *epigraph* of a curve in R^2, $y = f(x)$, $x \in [a, b]$, is the set defined as $\text{epig}(f) \equiv \{(x, y) \mid x \in [a, b] \land y \geq f(x)\}$. A curve is said to be convex iff its epigraph is convex. A curve is said to be *concave* iff $-f(x)$ is convex.

Theorem: A curve, $y = f(x)$, $R \mapsto R$, that is continuously differentiable and has monotonically increasing first derivative is convex.

Theorem: The convex hull of a finite set of points, V, is the set of all convex combinations of points of V, that is, if $V = \{x^i, i = 1 \ldots n\}$, then $\text{ch}(V) = \{x \mid x = [x^1, \ldots x^n]l, l \geq 0, \mathbf{1}'l = 1\}$.

A (non-linear) *constraint*, in R^n, is an inequality of the form $g(x) \leq 0$, $g : R^n \mapsto R$. The *feasible region* defined by m constraints, $g(x) \leq 0$, $g : R^n \mapsto R^m$, is the set of feasible (or viable) points $\{x \mid g(x) \leq 0\}$. At the feasible point x, the constraint $g_i(x)$ is said to be *active* or *tight* if the equality, $g_i(x) = 0$, holds, and it is said to be *inactive* or *slack* if the strict inequality, $g_i(x) < 0$, holds.

Polyedra

A *polyedron* in R^n is a feasible region defined by *linear constraints*: $Ax \leq d$. We can always compose an equality constraint, $a'x = \delta$ with two inequality constraints, $a'x \leq \delta$ e $a'x \geq \delta$.

Theorem: Polyedra are convex, but not necessarily bounded.

A *face* of dimension k, of a polyedron in R^n with m equality constraints, is a feasible region that obeys tightly to $n - m - k$ of the polyedron's inequality constraints. Equivalently, a point that obeys to r active inequality constraints is at a face of dimension $k = n - m - r$. A *vertex* is a face of dimension 0. An *edge* is a face of dimension 1, An *interior point* of the polyedron has all inequality constraints slack or inactive, that is, $k = n - m$. A *facet* is a face of dimension $k = n - m - 1$.

It is possible to have a point in a face of negative dimension. For example, Figure D.1 shows a point where $n - m + 1$ inequality constraints are active. This point is "super determined", since it is a point in R^n that obeys to $n+1$ equations, m equality constraints and $n - m + 1$ active inequality constraints. Such a point is said to be *degenerate*. From now on we assume the *non-degenerescence hypothesis*, stating that such points do not exist in the optimization problem at hand. This hypothesis is very reasonable, since the slightest perturbation to a degenerate problem transforms a degenerate point into one or more vertices, see Figure D.1.

A polyedron in *standard form*, $P_{A,d} \subset R^n$, is defined by n *signal constraints*, $x_i \geq 0$, and $m < n$ *equality constraints*, that is,

$$P_{A,d} = \{x \geq 0 \mid Ax = d\} \quad , \quad A \; m \times n$$

We can always rewrite a polyedron in standard form (at a higher dimensional space) using the following artifices:

1. Replace an unconstrained variable, x_i by the difference of two positive ones, $x_i^+ - x_i^-$ where $x_i^+ = max\{0, x_i\}$ e $x_i^- = max\{0, -x_i\}$.

2. Add a *slack variable*, $\chi \geq 0$ to each

   inequality

$$a'x \leq \delta \iff \begin{bmatrix} a & 1 \end{bmatrix} \begin{bmatrix} x \\ \chi \end{bmatrix} = \delta \quad .$$

From the definition of vertex we can see that, in a polyedron in standard form, $P_{A,d}$, a vertex is a feasible point where $n - m$ constraints are active. Hence, $n - m$ variables are null; these are the *residual variables* of this vertex. Let us permute the vector x so to place the residual variables at the last $n - m$ positions. Hence, the remaining (non-null) variables, the *basic variables* will be at the first m positions. Applying the same

permutation to the columns of matrix A, the block of the first m columns is called the *basis*, B, of this vertex, while the block of the remaining $n - m$ columns of A is called the *residual matrix*, R. That is, given vectors b and r with the basic and residual indices, the permuted matrix A can be partitioned as

$$\begin{bmatrix} A^b & A^r \end{bmatrix} = \begin{bmatrix} B & R \end{bmatrix}$$

In this form, it is easy to write the non-null variables explicitely,

$$\begin{bmatrix} x_b \\ x_r \end{bmatrix} \geq 0 \mid \begin{bmatrix} B & R \end{bmatrix} \begin{bmatrix} x_b \\ x_r \end{bmatrix} = d \text{ hence,}$$

$$x_b = B^{-1} [d - Rx_r]$$

Equating the residual variables to zero, it follows that

$$x_b = B^{-1} d \quad .$$

From the definition of degenerescence we see that the vertex of a polyedron in standard form is degenerate iff it has a null basic variable.

D.2 Linear Programming

This section presents Linear Programming, the simplest optimization problem studied in multi-dimensional mathematical programming. The simple structure of LP allows the formal development of relatively simple solution algorithms, namely, the primal and dual simplex. This section also presents some decomposition techniques used for solving LP problems in special forms.

D.2.1 Primal and Dual Simplex Algorithms

A LP problem in standard form asks for the minimum of a linear function inside a polyedron in standard form, that is,

$$\min \ cx, \quad x \geq 0 \mid Ax = d \quad .$$

Assume we know which are the residual (zero) variables of a given vertex. In this case we can form basic and residual index vectors, b and r, and obtain the basic (non-zero) variables of this vertex. Permuting and partitioning all objects of the LP problem according to the order established by the basic and residual index vectors, the LP problem is written as

$$\min \ \begin{bmatrix} c^b & c^r \end{bmatrix} \begin{bmatrix} x_b \\ x_r \end{bmatrix}, \quad x \geq 0 \mid \begin{bmatrix} B & R \end{bmatrix} \begin{bmatrix} x_b \\ x_r \end{bmatrix} = d \quad .$$

using the notation

$$\tilde{d} \equiv B^{-1}d \text{ and } \tilde{R} \equiv B^{-1}R ,$$

the basic solution corresponding to this vertex is $x_b = \tilde{d}$ (and $x_r = 0$).

Let us now proceed with an analysis of the sensitivity of this basic solution by a perturbation of a single residual variable. If we change a single residual variable, say the j-th element of x_r, allowing it to become positive, that is, making $x_{r(j)} > 0$, the basic solution, x_b becomes

$$\begin{aligned} x_b &= \tilde{d} - \tilde{R}x_r \\ &= \tilde{d} - x_{r(j)}\tilde{R}^j \end{aligned}$$

This solution remains feasible as long as it remains non-negative. Using the non-degeneregescence hypothesis, $\tilde{d} > 0$, and we know that it is possible to increase the value of $x_{r(j)}$, while keeping the basic solution feasible, up to a threshold $\epsilon > 0$, when some basic variable becomes null.

The value of this prturbed basic solution is

$$\begin{aligned} cx &= c^b x_b + c^r x_r \\ &= c^b B^{-1}[d - Rx_r] + c^r x_r \\ &= c^b \tilde{d} + (c^r - c^b \tilde{R})x_r \\ &\equiv \varphi - zx_r \\ &= \varphi - z^j x_{r(j)} \end{aligned}$$

Vector z is called the *reduced cost* of this basis.

The sensitivity analysis suggests the following algorithm used to generate a sequence of vertices of decreasing values, starting from an initial vertex, $[x_b \,|\, x_r]$.

Simplex Algorithm:

1. Find a residual index j, such that $z^j > 0$.

2. Compute, for $k \in K \equiv \{l \mid \tilde{R}_l^j > 0\}$, $\quad \epsilon_k = \tilde{d}_k / \tilde{R}_k^j$, and take $i \in \text{Argmin}_{k \in K} \ \epsilon_k$, i.e. $\epsilon(i) = \min_k \epsilon_k$.

3. Make the variable $x_{r(j)}$ basic, and $x_{b(i)}$ residual.

4. Go back to step 1.

The simplex can not proceed if $z \leq 0$ at the first step, or if, at the second step, the mimimum is taken over the empty set. In the second case the LP problem is unbounded. In the first case the current vertex is an optimal solution!

Changing the status basic / residual of a pair of variables is, in the LP jargon, *to pivot*. After each pivoting operation the basis inverse needs to be recomputed, that is, the basis needs to be *reinverted*. Numerically efficient implementation of the Simplex do not actually keep the basis inverse, instead, the basis inverse is represented by a numerical factorization, like $B = LU$ or $B = QR$. At each pivot operation the basis is changed by a single column, and there are efficient numerical algorithms used to update the numerical factorization representing the basis inverse, see Murtagh (1981) and Stern (1994).

Example 1: Let us illustrate the Simplex algorithm solving the following simple example.

Let us consider the LP problem $\min[-1, -1]x, \ 0 \le x \le 1$.
This problem can be restated in standard form:

$$c = \begin{bmatrix} -1 & -1 & 0 & 0 \end{bmatrix} \quad A = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \end{bmatrix} \quad d = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

The initial vertex $x = [0, 0]$ is assumed to be known.
Step 1: $r = [1, 2], \ b = [3, 4], \ B = A(:, b) = I, \ R = A(:, r) = I,$
$-z = c^r - c^b \tilde{R} = [-1, -1] - [0, 0] \Rightarrow z = [1, 1], \ j = 1, \ r(j) = 1,$
$x_b = \tilde{d} - \epsilon \tilde{R}^j = \begin{bmatrix} 1 \\ 1 \end{bmatrix} - \epsilon \begin{bmatrix} 1 \\ 0 \end{bmatrix} \Rightarrow \epsilon^* = 1, \ i = 1, \ b(i) = 3$
Step 2: $r = [3, 2], \ b = [1, 4], \ B = A(:, b) = I, \ R = A(:, r) = I,$
$-z = c^r - c^b \tilde{R} = [0, -1] - [-1, 0] \Rightarrow z = [-1, 1], \ j = 2, \ r(j) = 2,$
$x_b = \tilde{d} - \epsilon \tilde{R}^j = \begin{bmatrix} 1 \\ 1 \end{bmatrix} - \epsilon \begin{bmatrix} 0 \\ 1 \end{bmatrix} \Rightarrow \epsilon^* = 1, \ i = 2, \ b(i) = 4$
Step 3: $r = [3, 4], \ b = [1, 2], \ B = A(:, b) = I, \ R = A(:, r) = I,$
$-z = c^r - c^b \tilde{R} = [0, 0] - [-1, -1] \Rightarrow z = [-1, -1] < 0$

Obtaining the initial vertex

In order to obtain an initial vertex, used to start the simplex, we can use the auxiliary LP problem,

$$\min \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} \ | \ \begin{bmatrix} x \\ y \end{bmatrix} \ge 0 \ \wedge \ \begin{bmatrix} A & \text{diag}(\text{sign}(d)) \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = d$$

An initial vertex for the auxiliary problem is given by $\begin{bmatrix} 0 & \text{abs}(d') \end{bmatrix}'$. If the auxiliary problem has an optimal solution of value zero, the optimal solution gives a feasible vertex for the original problem;

if not, the original problem is unfeasible.

Duality

Given an LP problem, called the *primal* LP problem, we define a second problem, the *dual* problem (of the primal problem). Duality theory establishes important relations between the solution of the primal LP and the solution of its dual.

Given a LP problem in *canonic* form,

$$\min \ cx \mid x \geq 0 \wedge Ax \geq d \ ,$$

its dual LP problem is defined as

$$\max \ y'd \mid y \geq 0 \wedge y'A \leq c \ .$$

The primal and dual problems in canonic form have an intuitive economical interpretation. The primal problem can be interpreted as the classic ration problem: A_i^j is the quantity of nutrient of type j found in one unit of aliment of type i. c^i is the cost of one unit of aliment i, and d_j the minimum daily need of nutrient j. The primal optimal solution is a nutritionally feasible ration of minimum cost. The dual problem can be interpreted as a manufacturer of synthetic nutrients, looking for the "market value" for its nutrients line. The manufacturer income per synthetic ration is the objective function to be maximized. In order to keep its line of synthetic nutrients competitive, no natural aliment should provide nutrients cheaper than the corresponding synthetic mixture, these are the dual problem's constraints. The optimal prices for the synthetic nutrients, y^* can also be interpreted as marginal prices, giving the differential price increment of aliment i by differential increase of its content of nutrient j. The correctness of these interpretations are demonstrated by the duality properties discussed next.

Lemma 1: The dual of the dual is the primal PL problem.

Proof: Just observe that the dual of the primal LP in canonic form is equivalent to

$$\min \ -y'd \mid y \geq 0 \wedge -y'A \geq -c \ .$$

This problem is again in canonic form, and can be immediately dualized, yielding a problem equivalent to the original LP problem.

Weak Duality Theorem: If x and y are, respectively, feasible solutions of the primal and dual problems, then there is a non-negative gap between their values as solutions of these problems, that is,

$$cx \geq y'd \ .$$

Proof: By feasibility, $Ax \geq d$ and $y \geq 0$. Hence, $y'Ax \geq y'd$. In the same way, $y'A \leq c$ and $x \geq 0$. Hence $y'Ax \leq cx$. Therefore, $cx \geq y'd$. QED.

Corollary 1: If we have a pair of feasible solutions, x for the primal LP problem and y for its dual, and their values as primal and dual solutions coincide, that is, $cx^* = (y^*)'d$, then both solutions are optimal.

Corollary 2: If the primal LP problem is unbounded, its dual is unfeasible.

As we could re-write any LP problem in standard for, we can re-write any LP problem in canonical form. Hence, from Lemma 1, we know that the duality relation is defined between pairs of LP problems, whatever the form they have been writen.

Lemma 2: Given a primal in standard form,

$$\min \ cx \mid x \geq 0 \wedge Ax = d \ ,$$

its dual is

$$\max \ y'd \mid y \in R^m \wedge y'A \leq c \ .$$

Theorem (Simplex proof of correctness):

We shall prove that the Simplex stops at an optimal vertex. At the Simplex halting point we have $z = -(c^r - c^b B^{-1} R) \leq 0$. Let us consider $y' = c^b B^{-1}$ as a candidate solution for the dual.

$$
\begin{aligned}
\begin{bmatrix} c^b & c^r \end{bmatrix} &- y' \begin{bmatrix} B & R \end{bmatrix} \\
&= \begin{bmatrix} c^b & c^r \end{bmatrix} - c^b B^{-1} \begin{bmatrix} B & R \end{bmatrix} \\
&= \begin{bmatrix} c^b & c^r \end{bmatrix} - c^b \begin{bmatrix} I & \tilde{R} \end{bmatrix} \\
&= \begin{bmatrix} c^b & c^r \end{bmatrix} - \begin{bmatrix} c^b & c^b \tilde{R} \end{bmatrix} \\
&= \begin{bmatrix} 0 & -z \end{bmatrix} \geq 0
\end{aligned}
$$

Hence, y é is a feasible dual solution. Moreover, its value (as a dual solution) is $y'd = c^b B^{-1} d = c^b \tilde{d} = \varphi$, and, by corollary 1, both solutions are optimal.

Theorem (Strong Duality): If the primal problem is feasible and bounded, so is its dual. Moreover, the value of the primal and dual solutions coincide.

Proff: Constructive, by the Simplex algorithm.

Theorem (Complementary Slackness): Let x and y' be feasible solutions to a LP in standard form and its dual. These solutions are optimal iff $w'x = 0$, where $w = (c - y'A)$. The vectors x and w represent the slackness in the inequality constraints of the primal and dual LP problems. Since $x \geq 0$ and $w \geq 0$, the scalar product $w'x$ is null iff each

of its terms, $w_j x_j$, is null; or equivalently, if for each slack inequality constraint in the primal, the corresponding inequality constraint in the dual is tight, and vice-versa. Hence the name complementary slackness.

Proof: If the solutions are optimal, we could have obtained them by the Simplex algorithm. As in the Simplex proof of correctness, let

$$(c - y'A)x = \begin{bmatrix} 0 & z \end{bmatrix} \begin{bmatrix} x_b \\ 0 \end{bmatrix} = 0$$

If $(c - y'A)x = 0$, then $y'(Ax) = cx$, or $y'd = cx$,

and by the first corollary of the weak duality theorem, both solutions are optimal.

General Form of Dualidade

The following are LP problem of the most general form and its dual. An asterisk, $*$, indicates an unconstrained sub-vector

The general Primal LP problem,

$$\min \begin{bmatrix} c\{1\} & c\{2\} & c\{3\} \end{bmatrix} \begin{bmatrix} x\{1\} \\ x\{2\} \\ x\{3\} \end{bmatrix} \qquad \begin{matrix} x\{1\} & \geq & 0 \\ x\{2\} & * & \\ x\{3\} & \leq & 0 \end{matrix} \quad \Bigg|$$

$$\begin{bmatrix} A\{^1_1\} & A\{^2_1\} & A\{^3_1\} \\ A\{^1_2\} & A\{^2_2\} & A\{^3_2\} \\ A\{^1_3\} & A\{^2_3\} & A\{^3_3\} \end{bmatrix} \begin{bmatrix} x\{1\} \\ x\{2\} \\ x\{3\} \end{bmatrix} \begin{matrix} \leq & d\{1\} \\ = & d\{2\} \\ \geq & d\{3\} \end{matrix}$$

and its Dual LP problem:

$$\max \begin{bmatrix} d\{1\}' & d\{2\}' & d\{3\}' \end{bmatrix} \begin{bmatrix} y\{1\} \\ y\{2\} \\ y\{3\} \end{bmatrix} \qquad \begin{matrix} y\{1\} & \leq & 0 \\ y\{2\} & * & \\ y\{3\} & \geq & 0 \end{matrix} \quad \Bigg|$$

$$\begin{bmatrix} A\{^1_1\} & A\{^2_1\} & A\{^3_1\} \\ A\{^1_2\} & A\{^2_2\} & A\{^3_2\} \\ A\{^1_3\} & A\{^2_3\} & A\{^3_3\} \end{bmatrix}' \begin{bmatrix} y\{1\} \\ y\{2\} \\ y\{3\} \end{bmatrix} \begin{matrix} \leq & c\{1\}' \\ = & c\{2\}' \\ \geq & c\{3\}' \end{matrix}$$

The following are some interesting special cases:

Primal: $\max cx \mid Ax \geq d \wedge x \geq 0$ Dual: $\min y'd \mid y'A \geq c \wedge y \leq 0$

Primal: $\max cx \mid Ax \leq d \wedge x \in R^n$ Dual: $\max y'd \mid y'A = c \wedge y \leq 0$

Dual Simplex Algorithm

The Dual Simplex algorithm is analogous to the standard Simplex, but it works caring a basis that is dual feasible, and works to achieve primal feasibility. The Dual Simplex is very useful in several situations in which we solve a LP problem, and subsequently have to alter some constraints, loosing primal feasibility. We work with a standard LP program and its dual,

$$P: \ \min cx \ , \ x \geq 0 \ Ax = d \quad \text{and} \quad D: \ \max y'd \ , \ y'A \leq c$$

In dual feasible basis, $y = c^b B^{-1}$ is a dual feasible solution, that is

$$
\begin{aligned}
& \begin{bmatrix} c^b & c^r \end{bmatrix} - y' \begin{bmatrix} B & R \end{bmatrix} \\
&= \begin{bmatrix} c^b & c^r \end{bmatrix} - c^b B^{-1} \begin{bmatrix} B & R \end{bmatrix} \\
&= \begin{bmatrix} c^b & c^r \end{bmatrix} - c^b \begin{bmatrix} I & \tilde{R} \end{bmatrix} \\
&= \begin{bmatrix} c^b & c^r \end{bmatrix} - \begin{bmatrix} c^b & c^b \tilde{R} \end{bmatrix} \\
&= \begin{bmatrix} 0 & -z \end{bmatrix} \geq 0
\end{aligned}
$$

Now, let us rewrite the dual in a form that is analogous to the standard form, adding slack variables and using a partition of the coefficient matrix, $[B, R]$, as follows:

$$
\begin{aligned}
\max d'y \quad & A'y \leq c' \\
\max d'y \quad & \begin{bmatrix} B' \\ R' \end{bmatrix} y \leq \begin{bmatrix} c^{b'} \\ c^{r'} \end{bmatrix} \\
\max d'y \quad & \begin{bmatrix} B' & I & 0 \\ R' & 0 & I \end{bmatrix} \begin{bmatrix} y \\ w_b \\ w_r \end{bmatrix} = \begin{bmatrix} c^{b'} \\ c^{r'} \end{bmatrix} \ , \ w \geq 0
\end{aligned}
$$

In this form, the dual basis, its inverse, and corresponding basic solution are given by,

$$
\begin{bmatrix} B' & 0 \\ R' & I \end{bmatrix} , \begin{bmatrix} B^{-t} & 0 \\ -R'B^{-t} & I \end{bmatrix}
$$

$$
\begin{bmatrix} y \\ w_r \end{bmatrix} = \begin{bmatrix} B^{-t} & 0 \\ -R'B^{-t} & I \end{bmatrix} \begin{bmatrix} c^{b'} \\ c^{r'} \end{bmatrix} - \begin{bmatrix} B^{-t} & 0 \\ -R'B^{-t} & I \end{bmatrix} \begin{bmatrix} I \\ 0 \end{bmatrix} w_b \ \text{ i.e.}
$$

$$
y = B^{-t} c^{b'} - B^{-t} w_b \quad e \quad w_r = c^{r'} - R'B^{-t}c^{b'} + R'B^{-t}w_b
$$

Note that the indices in b and r correspond to basic and residual indices in the primal, the situation being reversed in the dual. As in the standard Simplex, we can increase a zero element of the residual vector in order to have a better dual solution,

$$d'y = d'B^{-t}(c^{b'} - w_b) = \text{const} - \tilde{d}'w_b$$

If $\tilde{d} \geq 0$ the primal basic solution is feasible, and we have the optimal solutions for both the primal and the dual problems. If there is an element $\tilde{d}_i < 0$, we can increase the value of the dual solution increasing $w_{b(i)}$. We can increase $w_{b(i)} = \nu$, without loosing dual feasibility, as long as we maintain

$$w_r = c^{r\prime} - R'B^{-t}c^{b\prime} + \nu R'B^{-t}I^i \geq 0 \ \text{ transposing}$$

$$c^r - \tilde{c}^b R + \nu B_i^{-1}R \geq 0 \ \text{ i.e.}$$

$$-z + \nu \tilde{R}_i \geq 0$$

Making $j = \arg\min\{\nu(j) = z^j/\tilde{R}_i^j \ , \ j \ | \ \tilde{R}_i^j < 0\}$, we have the index that leaves the dual basis. Hence, in the new list of indices b, that are primal basic, we can exclude $b(i)$, include $r(j)$, update the basis' inverse and proceed to a new dual simplex iteration, until we reach dual optimality or, equivalently, primal feasibility.

D.2.2   Decomposition Methods

Suppose we have a LP problem in the form

$$\min cx, \ x \geq 0 \,|\, Ax = b, \quad \text{where the matrix } \ A = \begin{bmatrix} \dot{A} \\ \ddot{A} \end{bmatrix} ,$$

and the polyedron described by $\ddot{A}x = \ddot{b}$ has a very "simple" structure, while $\dot{A}x = \dot{b}$ implies only a "few" additional constraints that, unfortunately, greatly complicate the problem.

For example, let $\ddot{A}x = \ddot{b}$ describe a set of separate LP problems, while $\dot{A}x = \dot{b}$ imposes global constrains coupling the variables of the several LP problems. This structure is known as Row Block Angular Form (RBAF), see section 5.2.

We now study the Danzig-Wolf method, that allow us to solve the original LP problem, by successive iterations between a "small" *main* or *master* problem, and a large but "simple" *subproblem* or *slave* problem. We assume that the simple polyedron is bounded, hence being the convex hull of its vertices

$$\ddot{X} = \{x \geq 0 \ | \ \ddot{A}x = \ddot{b}\} = ch(V) = Vl \ , \ l \geq 0 \ | \ \mathbf{1}'l = 1 \ .$$

The origianl LP problem is equivalent to the following master problem:

$$M: \ \ \min cVl \ , \ l \geq 0 \ | \ \begin{bmatrix} \dot{A}V \\ \mathbf{1}' \end{bmatrix} l = \begin{bmatrix} \dot{b} \\ 1 \end{bmatrix}$$

obviously this representation has only theoretical interest, for it is not practical to find the many vertices of V. A given basis B is optimal iff

$$-z = [cV]_R - ([cV]_B B^{-1})R \equiv [cV]_R - [y, \gamma]R \geq 0 \ .$$

This condition is equivalent of having, for any residual index, j,

$$cV^j - [y, \gamma] \begin{bmatrix} \dot{A}V^j \\ 1 \end{bmatrix} \geq 0 \text{ , or}$$

$$\gamma \leq cV^j - y\dot{A}V^j = (c - y\dot{A})V^j \text{ , or}$$

$$\gamma \leq \min(c - y\dot{A})v \text{ , } v \in \ddot{X}$$

Hence, we define the o sub-problem

$$S: \quad \min(c - y\dot{A})v \text{ , } v \geq 0 \mid \ddot{A}v = \ddot{b}$$

If the optimal solution of S, v^* has optimal value $(c - y\dot{A})v^* \geq \gamma$, the basis B is optimal for M. If not, v^* give us the next column for entering the basis, $\begin{bmatrix} \dot{A}v^* \\ 1 \end{bmatrix}$.

The optimal solution of the auxiliary problem also give us a lower bound for the original problem. Let x be any feasible solution for the original problem, that is, $x \in \ddot{X} \mid \dot{A}x = \dot{b}$. Since x is more constrained, $(c - y\dot{A})x \geq (c - y\dot{A})v^*$, hence, $cx \geq y\dot{b} + (c - y\dot{A})v^*$. Note that $y\dot{b}$ is the current upper bound. Also note that it is not necessary to have a monotonic increase in the lower bound. Hence we must keep track of the best lower bound found so far.

As we have seen, the Danzig-Wolf works very well for LP problems in RBAF. If we had a problem in CBAF - Column Block Angular Form, we could use Danzig-Wolf decomposition method on the problem's dual. This is essentially Benders decomposition method, that can be efficiently implemented using the Dual Simplex algorithm.

Exercises

1. Geometry and simple lemmas:

   a- Draw the simplex, S_n, and the cube, C_n of dimension 2 and 3. $S = \{x \geq 0 \mid \mathbf{1}'x \leq 1\}$, $C = \{x \geq 0 \mid Ix \leq \mathbf{1}\}$.

   b- Rewrite S_2, S_3, C_2 and C_3 as standard form plyedra in R^n, where $n = 3, 4, 4, 6$, respectively.

   c- Prove that a polyedron (in standard form) is convex.

   d- Prove duality lemmas 1 and 2.

   e- Prove that a bounded polyedron is the set of convex combinations of its vertices.

2. Write a program to solve a LP problem in standard form by exhaustive enumeration of its vertices. Suggestion: Write a function to enumerate all arrangements, $b = [b(1), \ldots b(m)]$, of m indices from $1 : n$, in increasing order that is, $b(j) > b(i)$ for

$j > i$. For each arrangement, b form the basis $B = A^b$. Check if B is invertible and, if so, check if the basic solution is a vertex, that is, if it is feasible, $\tilde{d} = B^{-1}d > 0$. Compute the value of all feasible basic solutions, and select the best one.

3. Adapt the Simplex algorithm to use the QR factorization of the basis. Explain how to update the factorization after a pivoting operation.

4. Adapt and implement the Simplex for LP problems with box constraints, that is

$$\min cx , \ l \leq x \leq u \ | \ Ax = d .$$

Hint: Consider a given feasible basis, B, and a partition $\begin{bmatrix} B & R & S \end{bmatrix}$, where $l_b < x_b < u_b,\ x_r = l_r,\ x_s = u_s,$ so that,
$x_b = B^{-1}d - B^{-1}Rx_r - B^{-1}Sx_s$ and
$cx = c^b B^{-1}d + (c^r - c^b B^{-1}R)x_r + (c^s - c^b B^{-1}S)x_s = \varphi + z^r x_r + z^s x_s$

If $z^{r(k)} < 0$, we can improve the current solution increasing this residual variable residual at its lower bound, $x_{r(k)} = l_{r(k)} + \delta_{r(k)},$ making
$x_b = B^{-1}d - B^{-1}Rl_r - B^{-1}Su_s - \delta_{r(k)}B^{-1}R^k$.
However, $\delta_{r(k)}$ shall respect the following bounds:
1- $x_{r(k)} = l_{r(k)} + \delta_{r(k)} \leq u_{r(k)},$ 2- $x_b \geq l_b,$ 3- $x_b \leq u_b$.
In a similar way, if $z^{s(k)} > 0$, we can improve the current solution decreasing this residual variable at its upper bound, $x_{s(k)} = u_{s(k)} - \delta_{s(k)}$.

5. Adapt and implement the Dual Simplex for LP problems with box constraints.

6. Implement Danzig-Wolf decomposition methods for RBAF problems.

D.3   Non-Linear Programming

Optimality and Lagrange Multipliers

We start this section giving an intuitive explanation of Lagrange's optimality conditions for a Non-Linear Programming (NLP) problem, given as

$$\min f(x),\ x \mid g(x) \leq 0 \wedge h(x) = 0 ,\ f : R^n \mapsto R ,\ g : R^n \mapsto R^m ,\ h : R^n \mapsto R^k .$$

We can imagine the function f as *potential*, or the "height" of a surface. An *equipotential* is a manifold where the function is constant, $f(x) = c$. The gradient

$$\nabla f \equiv \partial f / \partial x = \begin{bmatrix} \partial f / \partial x_1, & \partial f / \partial x_2, & \dots & \partial f / \partial x_n \end{bmatrix}$$

gives steepest ascent direction of the function at point x. Hence, the gradient $\nabla f(x)$ is orthogonal to the equipotential at this point.

Imagine a particle being "pulled down" by the force $-\nabla f(x)$. The optimal solution must be a point of equilibrium for the particle. Hence, either the force pulling the particle down is null, or else the force must be equilibrated by "reaction" forces exercised by the constraints. The reaction force exercised by an inequality constraint $g_i(x) \leq 0$, must obey the following conditions:

a) Be a force orthogonal to the equipotential curve of this constraint (since only the value of $g_i(x)$ is relevant for this constraint);

b) Be a force pulling the particle "inwards", that is, to the inside of the feasible region;

c) Moreover, a inequality constraint can only exercise a reaction force if it is tight, otherwise there is a slack allowing the particle to move even closer to this constraint.

An equality constraint, $h_i(x) = 0$, can be seen as a pair of inequality constraints, $h_i(x) \leq 0$ and $h_i(x) \geq 0$, but unlike an inequality constraint, an equality constraint is always active.

Our intuitive discussion can be summarized analytically by the following conditions known as *Lagrange's optimality conditions*:

If $x^* \in R^n$ é is an optimal point, then

$$\exists u \in R^m \ , \ v \in R^k \ \mid u\nabla g(x^*) + v\nabla h(x^*) - \nabla f(x^*) = 0 \ , \ \text{onde} \ \ u \leq 0 \wedge ug(x^*) = 0 \ .$$

The condition $u \leq 0$ implies that the inequality's reaction force points to the inside of the feasible region, while the *complementarity condition*, $ug = 0$, implies that only active constraints can exercise reaction forces. The vectors u and v are known as *Lagrange multipliers*.

Quadratic Programming

As an example, let us derive the Lagrange optimality conditions for Quadratic Programming (QP). QP is an important problem in its own right, and is also frequently used as a subproblem in methods designed to solve more general problems like, for example, Sequential Quadratic Programming, see Luenberger (1984) and Minoux and Vajda (1986).

The QP problem with linear constraints is stated as

$$min f(x) \equiv (1/2)x'Qx - \eta p'x \mid x \geq 0 \wedge Te * x = te \wedge Tl * x \leq tl$$

where the matrix dimensions are $Te \ me \times n$, $me < n$, $Tl \ ml \times n$, $ml < n$, $Ml = 1, 2, \ldots ml$, $Me = 1, 2, \ldots me$, $N = 1, 2, \ldots n$. We assume that the quadratic form defining the problem is symmetric and positive definite, that is, $Q = Q'$, $Q > 0$.

In the QP problem above, the objective function's gradient is

$$\nabla f = x'Q - \eta p' \ ,$$

and the gradients of the constraint functions are

$$g_i(x) = T_i x \leq t_i \Rightarrow \nabla g_i = T_i \ .$$

Hence, the Lagrange optimality conditions are

$$x \in R_+^n, s \in R_+^n, l \in R_+^{ml}, e \in R^{me}, \quad | \quad -(x'Q - \eta p') + s' - l'Tl + e'Te = 0$$

$$\wedge \ \forall i \in N \ , \ x_i s_i = 0 \ \wedge \ \forall k \in Ml \ , \ (Tl * x - tl)_k l_k = 0 \ \text{ or}$$

$$x \in R_+^n, s \in R_+^n, l \in R_+^{ml}, e \in R^{me}, y \in R_+^{ml} \quad | \quad Qx - s' + Tl' * l + Te'e = \eta p$$

$$\wedge \ \forall i \in N \ , \ x_i s_i = 0 \ \wedge \ \forall k \in Ml \ , \ yl_k l_k = 0 \ \text{ onde } yl = (tl - Tl * x)$$

The Complementarity Conditions (CC), $x's = 0$ e $yl'l = 0$, indicate that only active constraints can help to equilibrate non-negative components of the objective function's gradient. Using the change of variables $e = ep - em$, ep, $em \geq 0$, the optimal solution is characterized by the optimality and feasibility conditions

$$\begin{bmatrix} x \\ l \\ ep \\ en \\ s \\ yl \end{bmatrix} \geq 0 \ | \ \begin{bmatrix} Tl & 0 & 0 & 0 & 0 & I \\ Te & 0 & 0 & 0 & 0 & 0 \\ Q & Tl' & Te' & -Te' & -I & 0 \end{bmatrix} \begin{bmatrix} x \\ l \\ ep \\ en \\ s \\ yl \end{bmatrix} = \begin{bmatrix} tl \\ te \\ \eta p \end{bmatrix}$$

$$x's = 0, \ yl'l = 0.$$

Observe the formal resemblance of the last feasibility and optimality conditions to a LP in standard form where the non-linearity of the problem is encapsulated in the complementarity conditions. These observations are the key to adapt the Simplex to solve a QP, see Stern et al. (2006) and Wolfe (1959). This approach leads to efficient algorithms for *Parametric Quadratic Programming* and the computation of *Efficient Frontiers*, see Alexander and Francis (1986) and Markowitz (1952, 1956, 1987).

D.3.1 GRG: Generalized Reduced Gradient

Let us consider a NLP problem with non-linear equality constraints, plus box constraints over the variables' range,

$$\min f(x) \ , \quad f : R^n \mapsto R$$

$$l \leq x \leq u \ | \ h(x) = 0 \ , \quad h : R^n \mapsto R^m$$

The Generalized Reduced Gradient (GRG) method emulates the behaiviour of the Simplex method, for a local linearization of the NLP problem, see Abadie and Carpentier

(1969) and Minoux and Vajda (1986), for an intuitive presentation see Himmelblau (1972). Let x be an initial feasible point. As for LP, we assume a non-degenerescence hypothesis, that is, we assume that, at a given feasible point, a maximum of $(n - m)$ box constraints can be active. Hence, we can take m of the variables with slack box constraints as basic (or dependent) variables, and the remaining $n - m$ variables as residual (or independent) variables. As in the Simplex algorithm, we permute and partition all vector and matrix objects to better display this distinction,

$$x = \begin{bmatrix} x_b \\ x_r \end{bmatrix} , \quad l = \begin{bmatrix} l_b \\ l_r \end{bmatrix} , \quad u = \begin{bmatrix} u_b \\ u_r \end{bmatrix} , \quad \nabla f(x) = \begin{bmatrix} \nabla^b f(x) & \nabla^r f(x) \end{bmatrix}$$

$$J(x) = \begin{bmatrix} J^B(x) & J^R(x) \end{bmatrix} = \begin{bmatrix} \nabla^b h_1(x) & \nabla^r h_1(x) \\ \nabla^b h_2(x) & \nabla^r h_2(x) \\ \vdots & \vdots \\ \nabla^b h_m(x) & \nabla^r h_m(x) \end{bmatrix}$$

Let us consider the effect of a small alteration to the current feasible point, $x + \delta$, assuming that the functions f and h are continuous and differentiable. The corresponding alteration to the solution's value is

$$\Delta f = f(x + \delta) - f(x) \approx \nabla f(x) \, \delta = \begin{bmatrix} \nabla^b f(x) & \nabla^r f(x) \end{bmatrix} \begin{bmatrix} \delta_b \\ \delta_r \end{bmatrix}$$

We also want the altered solution, $x + \delta$, to remain (approximately) feasible, that is,

$$\Delta h = h(x + \delta) - h(x) \approx J(x) \, \delta = \begin{bmatrix} J^b(x) & J^r(x) \end{bmatrix} \begin{bmatrix} \delta_b \\ \delta_r \end{bmatrix} = 0$$

Isolating δ_b, and assuming that the basis $J^b(x)$ is invertible,

$$\begin{aligned} \delta_b &= -\left(J^b(x)\right)^{-1} J^r(x) \, \delta_r \\ \Delta f &\approx \nabla^b f(x) \, \delta_b + \nabla^r f(x) \, \delta_r \\ &= \left(\nabla^r f(x) - \nabla^b f(x) \left(J^b(x)\right)^{-1} J^r(x)\right) \delta_r = z(x) \, \delta_r \end{aligned}$$

Since the problem is non-linear, we can not assure that an optimal solution has all residual variables with one active constraint, that is, are at one side of the box, as in a standard LP problem. Therefore, there is no motivation to restrict δ_r to have only one non-zero component, as in the Simplex. Instead, we suggest to move the current solution (in the space of residual variables) along the direction given by the vector v_r, opposed to the reduced gradient, as long as the corresponding box constraint is slack, that is,

$$v_{r(i)} = \begin{cases} -z^i & \text{if } z^i > 0 \text{ and } x_{r(i)} > l_{r(i)} \\ -z^i & \text{if } z^i < 0 \text{ and } x_{r(i)} < u_{r(i)} \\ 0 & \text{otherwise} \end{cases}$$

In subsection D.3.4 shall we give general conditions that assure global convergence for NLP algorithms, and we will see that the discontinuity of vector v_r as a function of the box constraints slacks is undesirable. Hence, we shall use a continuous version of the search direction like, for example,

$$v_{r(i)} = \begin{cases} -\gamma(x_{r(i)} - l_{r(i)})z^i & \text{if } z^i > 0 \text{ and } x_{r(i)} > l_{r(i)} \\ -\gamma(u_{r(i)} - x_{r(i)})z^i & \text{if } z^i < 0 \text{ and } x_{r(i)} < u_{r(i)} \\ 0 & \text{otherwise} \end{cases}$$

where $\gamma(x) = x/\epsilon$, if $0 \le x \le \epsilon$; and $\gamma(x) = 1$, otherwise .

The basic idea of one iteration of the GRG method is to move the feasible point by a step $x + \delta$ with $\delta = \eta v$, where $v_b = -\left(J^b(x)\right)^{-1} J^r(x) v_r$, that is, a step (in the space of residual variables) of size η in the direction v_r. In order to determine the step size, η, we need to perform a line search, always respecting the box constraints.

Note that the direction, in the space of basic variables, v_b, has been chosen so that $x + \eta v$, remains (approximately) feasible, since we are moving inside a hyperplane that is tangent to the algebraic manifold defined by $h(x) = 0$. The new nearly feasible point, x, shall then receive a correction Δx in order to regain exact feasibility for the non-linear constraints, that is, so that $h(x + \Delta x) = 0$. The nearly feasible point x can be used a the starting point for a recursive method used to get exact feasiblity, like the Newton-Raphson method, that uses the basic Jacobian, $J^b(x)$, to compute the correction

$$\Delta x_b = -\left(J^b(x)\right)^{-1} h(x_b, x_r) .$$

D.3.2   Line Search and Local Convergence

This section analyses the problem of minimizing an unidimensional function, $f(x)$. First, let us consider the problem of finding the root (zero) of a differentiable function, approximated by its first order Taylor expansion, $g(x) \approx q(x^k) + g'(x^k)(x - x^k)$. This approximation implies that $g(x^{k+1}) \approx 0$, where

$$x^{k+1} = x^k - g'(x^k)^{-1}g(x^k)$$

This is Newton's method, used to find the root of an unidimensional function.

If a function $f(x)$ is differentiable, its minimum is at a point where the function's first derivative is null. Hence, we can use Newton's method for minimizing $f(x)$,

$$x^{k+1} = x^k - f''(x^k)^{-1}f'(x^k)$$

Let us examine how fast the sequence generated by Newton's method approaches the optimal solution, x^*, assuming the starting point, x^0, is already close enough to x^*. Assuming third order differentiability, we can write

$$0 = f'(x^*) = f'(x^k) + f''(x^k)(x^* - x^k) + (1/2)f'''(y^k)(x^* - x^k)^2 \text{ , or}$$

$$x^* = x^k - f''(x^k)^{-1} f'(x^k) - (1/2) f''(x^k)^{-1} f'''(y^k)(x^* - x^k)^2$$

Subtracting the equation that defines Newton's method, we have

$$(x^{k+1} - x^*) = (1/2) f''(x^k)^{-1} f'''(y^k) (x^k - x^*)^2$$

As we shall see in the following, this result implies that Newton's method converges very fast (quadratically), if we are already close enough to the optimal solution. However, Newton's method needs a lot of differential information about the function, something that may be hard to obtain. Moreover, far from the optimum, one can not be sure about the method's convergence. The following methods overcome these difficulties.

Let us now examine the Golden Ratio search method, for minimizing a unidimensional and unimodal function, $f(x)$, in the interval, $[x^1, x^4]$. Assume we know the function's value at four points, the extremes of the interval and two interior points, $x^1 < x^2 < x^3 < x^4$. From the unimodality hypothesis we can know that the point of minimum, x^*, is in one of the sub-itervals, that is

$$f(x^2) \leq f(x^3) \Rightarrow x^* \in [x^1, x^3] \quad , \quad f(x^2) > f(x^3) \Rightarrow x^* \in [x^2, x^4] \quad .$$

without loss of generality, let us consider the way to divide the interval $[0, 1]$. A ratio r defines a symmetric division in the form $0 < 1 - r < r < 1$. Dividing the subinterval $[0, r]$ by the same ratio r, we obtain the points $0 < r(1 - r) < r^2 < r$. We want the points r^2 and $1 - r$ to coincide, so that it will only be necessary to evaluate the function at one additional point, taht is, we want $r^2 + r - 1 = 0$. Hence, $r = (\sqrt{5} - 1)/2$, this is the *golden ratio* $r \approx 0.6180340$.

The golden ratio search method is robust, working for any unimodal function, and using only the function's value at the search points. However, the extremes of the size of the search interval decreases only linearly with the number of iterations.

Polynomial methods, studied next, try to conciliate the best characteristics of the methods already presented. Polynomial methods for minimizing an unidimensional function, $\min f(x + \eta)$, on $\eta \geq 0$, rely on a polynomial, $p(x)$, that locally approximates $f(x)$, and the subsequent minimization of the adjusted polynomial. The simplest of these methods is quadratic adjustment. Assume we know at three points, η_1, η_2, η_3, the respective function values, $f_i = f(x + \eta_i)$. Considering the equations for the interpolating polynomial

$$q(\eta) = a\eta^2 + b\eta + c \quad , \quad q(\eta_i) = f_i$$

we obtain the polynomial

$$a = \frac{f_1(\eta_2 - \eta_3) + f_2(\eta_3 - \eta_1) + f_3(\eta_1 - \eta_2)}{-(\eta_2 - \eta_1)(\eta_3 - \eta_2)(\eta_3 - \eta_1)}$$

$$b = \frac{f_1(\eta_3^2 - \eta_2^2) + f_2(\eta_1^2 - \eta_3^2) + f_3(\eta_2^2 - \eta_1^2)}{-(\eta_2 - \eta_1)(\eta_3 - \eta_2)(\eta_3 - \eta_1)}$$

$$c = \frac{f_1(\eta_2^2\eta_3 - \eta_3^2\eta_2) + f_2(\eta_3^2\eta_1 - \eta_1^2\eta_3) + f_3(\eta_1^2\eta_2 - \eta_2^2\eta_1)}{-(\eta_2 - \eta_1)(\eta_3 - \eta_2)(\eta_3 - \eta_1)}$$

Equating the first derivative of the interpolating polynomial to zero, $q'(\eta_4) = 2a\eta + b$, we obtain its point of minimum, $\eta_4 = a/2b$ or, directly from the function's values,

$$\eta_4 = \frac{1}{2}\frac{f_1(\eta_3^2 - \eta_2^2) + f_2(\eta_1^2 - \eta_3^2) + f_3(\eta_2^2 - \eta_1^2)}{f_1(\eta_3 - \eta_2) + f_2(\eta_1 - \eta_3) + f_3(\eta_2 - \eta_1)}$$

We should try to use the initial points in the "interpolating pattern" $\eta_1 < \eta_2 < \eta_3$ e $f_1 \geq f_2 \leq f_3$, that is, three points where the intermediary point has the smallest function's value. So doing, we know that the minimum of the interpolating polynomial is inside of the initial search interval, that is, $\eta_4 \in [\eta_1, \eta_3]$. In this situation we are interpolating and not extrapolating the function, favoring the numerical stability of the procedure.

Choosing η_4 and two more points from the initial three, we have a new set of three points in the desired interpolating pattern, and are ready to proceed for the next iteration. Note that, in general, we can not guaranty that η_4 is the best point in the new set of three. However, η_4 will always replace the worst point in the old set. Hence, the sum $z = f_1 + f_2 + f_3$ is monotonically decreasing. In section D.3.4 we shall see that these properties assure the global convergence of the quadratic adjustment line search algorithm.

Let us now consider the errors relative to the minimum argument, $\epsilon_i = x^* - x_i$. We can write $\epsilon_4 = g(\epsilon_1, \epsilon_2, \epsilon_3)$, where the function g is a second order polynomial. This is because η_4 is obtained by a quadratic adjustment, that is also symmetric in its arguments, since the order of the first three points is irrelevant. Moreover, it is nor hard to check that ϵ_4 is zero if two of the three initial errors are zero. Hence, close to the minimum, x^*, we have the following approximation for the forth error:

$$\epsilon_4 = C\left(\epsilon_1\epsilon_2 + \epsilon_1\epsilon_3 + \epsilon_2\epsilon_3\right)$$

Assuming that the process is converging, the k-th error is approximately $\epsilon_{k+4} = C\epsilon_{k+1}\epsilon_{k+2}$. Taking $l_k = \log(C^{1/2}\epsilon_k)$, we have $l_{k+3} = l_{k+1} + l_k$, with characteristic equation $\lambda^3 - \lambda - 1 = 0$. The largest root of this equation is $\lambda \approx 1.3$. This is the order of convergence of this method, as defined next.

We say that a sequence of real numbers $r^k \to r^*$ converges at least in order $p > 0$ if

$$0 \leq \lim_{k \to \infty} \frac{|r^{k+1} - r^*|}{|r^k - r^*|^p} = \beta < \infty$$

The sequence *order of convergence* is the supremum of constants $p > 0$ in such conditions. If $p = 1$ and $\beta < 1$, we say that the sequence has *linear convergence* with rate β. If $\beta = 0$, we say that the sequence has *super linear* convergence.

For example, for $c \geq 1$, c is the order of convergence of the sequence $a^{(c^k)}$. We can also see that $1/k$ converges in order 1, although it is not linearly convergent, because $r^{k+1}/r^k \to 1$. Finally, $(1/k)^k$ converges in order 1, because for any $p > 1$, $r^{k+1}/(r^k)^p \to \infty$, However, this convergence is super-linear, because $r^{k+1}/r^k \to 0$.

D.3.3   The Gradient ParTan Algorithm

In this section we present the method of Parallel Tangents, ParTan, developed by Shah, Buehler and Kempthorne (1964) for solving the problem of minimizing an unconstrained convex function.

Let us first review the definition of some geometric concepts like parallelism and orthogonality for (hyper)planes of arbitrary dimension. The following definitions refer to arbitrary vector subspaces, and may not coincide with some definitions used in tri-dimensional geometry. Two lines are parallel if they have the same direction. Two lines are orthogonal if the inner product of their directions is zero. A line is parallel to a plane if it is parallel to a line in this plane. A line is orthogonal to a plane if it is orthogonal to every line in this plane A plane is parallel to another plane if every line in this plane is parralel to the other plane. A plane is orthogonal to another plane if every line in this plane is orthogonal to the other plane.

The ParTan method, as so many others, rely on the idea of modeling the function to be minimized by a quadratic function. Without loss of generality, assume that this quadratic is centered at the origin, that is, $f(x) = (1/2)x'Qx$. Using the linear transformation $y = Ux$, where U is the Cholesky factor $U'U = Q$, we can rewrite f with spherical symmetry,

$$f(y) = (1/2)(U^{-1}y)'Q(U^{-1}y) = (1/2)y'(U^{-t}(U'U)U^{-1})y = (1/2)y'Iy$$

A fundamental property of an arbitrary linear transformation, $y = Ux$, is to preserve the properties of coplanarity and parallelism, that is,

- If the points $x^1 \ldots x^k$ belong to the same plane (line), so do the points $y^1 \ldots y^k$, and vice-versa.

- If the planes $\pi_{1,\ldots k}$ and $\pi_{k+1,\ldots k+h}$ determined, in the old coordinate system by the points $x^1 \ldots x^k$ and $x^{k+1} \ldots x^{k+h}$, are parallel, then the planes determined, in the new coordinate system, by the points $y^1 \ldots y^k$ and $y^{k+1} \ldots y^{k+h}$, are also parallel.

Therefore, if we define a good algorithm for the particular case of spherical functions, using only parallelism and coplanarity relations, then this algorithm remains valid in the general case. This is the fundamental idea used to develop the ParTan algorithm.

Finally, let us point out that orthogonality, $v'w = 0$, is a relation that is *not* preserved by linear transformations. If $v = Ux$ e $w = Uy$, then $v'w = (Ux)'(Uy) = x'(U'U)y = x'Qy$. Therefore we shall use the relation of Q-conjugacy, $x'Qy = 0$, or conjugacy for short if a quadratic form Q is understood from the context, as a generalization of the concept of orthogonality.

We use the following notation and nomenclature:
- p^k for an arbitrary point;

- q^k for the gradient of f in p^k, i.e., $q^k = Qp^k$;
- π_k for the plane tangent to the equipotential of f through p^k, i.e., for the plane containing p^k and orthogonal to q^k; and
- $\pi_{1,\ldots k}$ for the (hyper)plane of dimension $k-1$ determined by the points $p_1 \ldots p_k$. Hence, $\pi_{1,2}$ is a line, $\pi_{1,2,3}$ is a bidimensional plane, etc.
- We define the *conjugacy coefficient* $c_{k,j} \equiv (p^k)'Qp^j = (p^k)'q^j = c_{j,k}$.
- A line through a point p^k is said to be *degenerate* if it belongs to the plane π_k.

Let us first examine the geometry of the bidimensional case. Let $f(x) = (1/2)x'Qx$ be a given bidimensional quadratic function that, without loss of generality, we assume centered at the origin. The following geometric method can be used to find its minimum, p^*, see Figure D.2a.

Parallel Chords Algorithm:

1) Find the minimizing points, p^0 and p^3, on two parallel lines, r_0 and r_3.

2) Find the minimizing point, p^4, on the line $\pi_{0,3}$.

From the problem's spherical symmetry it is clear that the center, p^* belongs to the line $\pi_{0,3}$, so that p^4, the minimizer on $\pi_{0,3}$, is in fact the minimizer on the hole plane, p^*.

Since p^0 e p^3 are minimizers for $f(x)$ on the lines r_0 e r_3, these lines are also tangential to the respective equipotentials of f on p^0 and p^3, that is to say, p^0 and p^3 determine "parallel tangents". The following algorithm follows this idea:

Bidimensional ParTan Algorithm:

1) Take an arbitrary initial point, p^0.

2) Take p^2 the point of minimum on a non degenerate line, p^0

3) Take p^3 the point of minimum on the line through p^2 that is parallel to π_0.

4) Take p^4 the point of minimum on the line $\pi_{0,3}$.

In Figure D.2b we can see that, for spherical functions, this algorithm is just a particular form of implementing the parallel chords method. Since the coplanarity and parallelism relations (used to specify the algorithm) are invariant by linear transformations, the algorithm is correct for any quadratic function. Notice that the vectors $w^4 = p^4 - p^2$ and $w^2 = p^2 - p^0$ are orthogonal. Let us now extend this algorithm to the tridimensional space.

Tridimensional ParTan Algorithm:

1) Take an arbitrary initial point, p^0.

2) Take p^2 as the minimizer over a non degenerate line through p^0.

3) Take p^3 as the minimizer on a line through p^2, that is parallel to π_0 and non degenerate.
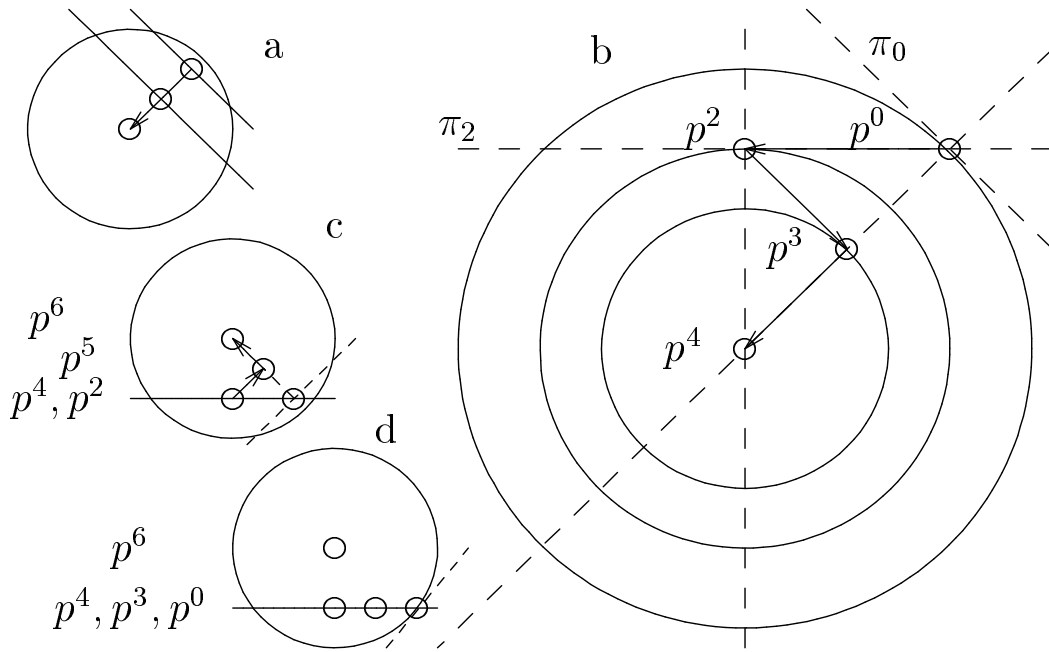
Figure D.2 Partan in a Sphere

4) Take p^4 as the minimizer on the line $\pi_{0,3}$.

5) Take p^5 as the minimizer on the line through p^4 parallel to the intersection of π_0 and π_2.

6) Take p^6 as the minimizer on the line $\pi_{2,5}$.

Let us prove that p^6 is indeed the optimal point, looking at the problem in the co-ordinate system where it has spherical symmetry, see Figure D.2. In order to check the optimality of p^6, we observe that:

1) $p^5 - p^4 \,//\, \pi_0 \cap \pi_2$, 2) $p^* - p^0 \perp \pi_0$ and $p^* - p^2 \perp \pi_2$, 3) $p^5 - p^4 \perp \pi_{0,2,*}$,
4) $p^5 - p^4 \perp \pi_{0,2}$, 5) $p^5 - p^4 \in \pi_{2,4,*}$, 6) $p^6 = p^*$.

The statements above a valid: 1) by construction, 2) by symmetry, 3) by 1 and 2, 4) because $\pi_{0,2} \in \pi_{0,2,*}$, 5) by symmetry, and 6) from the correctness of ParTan 2D.

We can make some further remarks on the geometry of ParTan 3D with spherical symmetry. First, we see that p^{2k} is the minimizer on plane $\pi_{0,2,\dots 2k}$. Second, we see that vector $w^{2k} \equiv p^{2k} - p^{2k-2}$ is perpendicular to this plane. Hence, the vectors w^{2k} are mutually orthogonal. These observations are the key for generalising the ParTan to n-dimensional space, and also to prove its correctness.

N-dimensional ParTan Algorithm:

1) Take an arbitrary initial point, p^0.

2) Take p^2 as the minimizer on a non-degenerate line through p^0.

3) For $k = 1, 2, \ldots n - 1$:

3a) Take p^{2k+1} as the minimizer on a line through p^{2k} that is non-degenerate and parallel to the planes $\pi_0, \pi_2, \ldots \pi_{2k-2}$.

3b) Take p^{2k+2} as the minimizer on the line through p^{2k-2} and p^{2k+1}.

In the n-dimensional ParTan, point p^{2k} is the minimizer of the objective function on a subspace of dimension k. Hence, the gradient q^{2k} is orthogonal to all previous search directions, that is,

$$(q^{2k})'w^{2k} = (q^{2k})'w^{2k-2} = \ldots = (q^{2k})'w^2 = 0$$

Also, $q^k = Qp^k$ and $w^{2k} = p^{2k} - p^{2k-2}$, so that the conjugacy coefficients $c_{2k,2j} = (p^{2k})'Qp^{2j}$ are all equal. Moreover, the ParTan algorithm requires that the vector $(p^{2k+1} - p^{2k})$ be parallel to the tangent planes π_{2j}, $j < k$, that is,

$$(q^{2j})'(p^{2k+1} - p^{2k}) = (p^{2j})'Q(p^{2k+1} - p^{2k}) = 0 , \quad j < k .$$

so that

$$(p^{2j})'Qp^{2k} = (p^{2j})'Qp^{2k+1} , \quad j = 0, 1, \ldots k - 1, \ k = 1, 2, \ldots n - 1 .$$

Subtracting the equations

$$(p^{k+2})'Qp^{2n} - (p^{k+2})'Qp^{2n-2} = 0 \ \text{ and } \ (p^k)'Qp^{2n} - (p^k)'Qp^{2n-2} = 0$$

we have

$$(p^{2k+2} - p^k)'Q(p^{2n} - p^{2n-2}) = (w^{2k})'Qw^{2n} = 0$$

that is, the vectors w^{2k}, $k = 1, \ldots n$, are all Q-conjugate.

A rigorous geometric proof, by induction on the dimension n, for the correctness of the ParTan algorithm can be found in Shah, Buehler and Kempthorne (1964), and ann intuitive presentation in Himmelblau (1972).

One of the observations made on our analysis of the ParTan algorithm was that p^{2k} is the mimimizer on the plane $\pi_{0,2,\ldots 2k}$. This observation give us a simple way of choosing the direction $p^{2k+1} - p^{2k}$, respecting the condition of being parallel to the planes $\pi_0, \pi_2, \ldots \pi_{2k-2}$. We can always choose the direction $p^{2k+1} - p^{2k}$ perpendicular to π_{2k}, that is, choose the gradient direction. The parallelism condition is satisfied because the three planes, π_{2k}, $\pi_{0,2,\ldots 2k}$ and $\pi'_{0,2,\ldots 2k}$, where the last is the plane parallel to the second going through the origin, are all parallel. All the gradients, $q^0, q^2, \ldots q^{2k-2}$ are in $\pi'_{0,2,\ldots 2k}$.

Hence, taking the gradient direction, q^{2k}, assures the orthogonality with the previous gradient directions, $q^0, q^2, \ldots q^{2k-2}$, satisfying the parallelism condition. This is the Gradient ParTan Algorithm.

The Gradient ParTan is a particular case of the ParTan Algorithm. It finds the optimal solution of a quadratic function in a finite number $(2n)$ of steps. This line of argument can be used to show that, if the quadratic model of the objective function is good, the ParTan algorithm converges quadratically. Nevertheless, even if the quadratic model for the objective function is poor, the even steps are Cauchy (steepest descent) steps. This explains the Gradient ParTan robustness as an optimization algorithm, even if it starts far away from the optimal solution.

The ParTan needs two line searches for each dimension, the even and odd steps. Far away from the optimal solution a Cauchy method would use only one line search. Close to the optimal solution alternative algorithms known as Conjugate Gradient algorithms, achieve quadratic convergence also using only one line search per dimension. Nevertheless, in order to use these algorithms one has to devise a monitoring system that keeps track of how well the quadratic model is doing, and use it to decide when to make the transition from the Cauchy to the Conjugate Gradient algorithm.

The Partanization of search directions often provides a simple mechanism to upgrade an algorithm based on Cauchy (steepest descent) line search steps, accelerating it to achieve quadratic convergence, while keeping the robustness that is so characteristic of Cauchy methods.

D.3.4 Global Convergence

In this section we give some conditions that assures global convergence for a NLP algorithm. We follow the ideas of Zangwill (1964), similar analyses are presented in Luenberger (1984) and Minoux and Vajda (1986).

We define an Algorithm as an iterative process generating a sequence of points, $x^0, x^1, x^2 \ldots$, that oby a recursion equation of the form $x^{k+1} \in A_k(x^k)$, where the *point-to-set map* $A_k(x^k)$ defines the possible successors of x^k in the sequence.

The idea of using an point-to-set map, instead of a ordinary function or point-to-point map, allows us to study in a unified way a hole class of algorithms, including alternative implementations of several details, approximate or inexact computations, randomized steps, etc. The basic property we look for on the maps defining an algorithm is *closure*, defined as follows.

A point-to-set map from space X to space Y, is *closed* at x if the following condition holds: If a sequence x^k converges to $x \in X$, and the sequence y^k converges to $y \in Y$,

where $y^k \in A(x)$, then the also the limit y is in the image $A(x)$, that is,

$$x^k \to x \ , \ y^k \to y \ , \ y^k \in A(x^k) \ \Rightarrow \ y \in A(x) \ .$$

The map is closed in $C \subseteq X$ if it is closed at any point of C. Note that if we replace, in the definition of closed map, the inclusion relation by the equality relation, we get the definition of continuity for point-to-point functions. Therefore, the closure property is a generalization of continuity. Indeed, a continuous function is closed, although the contrary is not necessarily true.

The basic idea of Zangwill's global convergence theorem is to find some characteristic that is continuously "improved" at each iteration of the algorithm. This characteristic is represented by the concept of *descendence function.*

Let A be an algorithm in X for solving the problem P, and let $S \subset X$ be the solution set for P. A function $Z(x)$ é is a descendence function for (X, A, S) if the composition of Z and A is always decreasing outside the solution set, and does not increase inside the solution set, that is,

$$x \notin S \wedge y \in A(x) \Rightarrow Z(y) < Z(x) \quad \text{and} \quad x \in S \wedge y \in A(x) \Rightarrow Z(y) \leq Z(x) \ .$$

In optimization problems, some times the very objective function is a good descendence function. Other times, more complex descendence functions have to be used, for example, the objective function with auxiliary terms, like penalties for constraint violations.

Before we state Zangwill's theorem, let us review two basic concepts of set topology: An *accumulation point* os a sequence is a limit point for one of its sub-sequences. A set is *compact* iff any (infinite) sequence has an accumulation point inside the set. In R^n, a set is compact if it is closed and bounded.

Zangwill's Global Convergence Theorem:

Let Z be a descendence function for the algorithm A defined in X with solution set S, and let $x^0, x^1, x^2, \dots$ be a sequence generated by this algorithm such that:
A) The map A is closed in any point outside S,
B) All points in the sequence remain inside a compact set $C \subseteq X$, and
C) Z is continuous.
Then, any accumulation point of the sequence is in the solution set.

Proof: From C compacity, a sequence generated by the algorithm has a limit point, $x \in C \subseteq X$, for a subsequence, $x^{s(k)}$. From the continuity of Z in X, the limit value of Z in the subsequence coincides withg the value of Z at the limit point, that is, $Z(x^{s(k)}) \to Z(x)$. But the complete sequence, $Z(x^k)$ is monotonically decreasing, hence, if $s(k) \leq j \leq s(k+1)$ then $Z(x^{s(k)}) \geq Z(x^j) \geq Z(x^{s(k+1)})$, and the value of Z in the complete sequence also converges to the value of Z at the accumulation point, that is $Z(x^k) \to Z(x)$.

Let us now imagine, for a proof by contradiction, that $Z(A(x)) < Z(x)$. Let us consider the sub-sequence of the successors of the points in the first sub-sequence, $x^{s(k)+1}$.

This second sub-sequence, again by compacity, also has an accumulation point, x'. But from the result in the last paragraph, the value of the descendence function in both sub-sequences converge to the limit value of the hole sequence, that is, $\lim Z(x^{s(k)+1}) = \lim Z(x^k) = \lim Z(x^{s(k)})$. So we have prooved the impossibility of x not being a solution.

Several algorithms are formulated as a composition of several steps. Hence, the map describing the hole algorithm is the composition of several maps, one for each step. A typical example would be a step for choosing a search direction, followed by a step for a line search. The following lemmas are useful in the construction of such composite maps.

First Composition Lemma: Let A from X to Y, and B from Y to Z, be point-to-set maps, A closed in $x \in X$, B closed in $A(x)$. If any sequence x^k converging to x, $y^k \in A(x^k)$ has an accumulation point y, then the composed map $B \circ A$ is closed in x.

Second Composition Lemma: Let A from X to Y, and B from Y to Z, be point-to set maps, A closed in $x \in X$, B closed in $A(x)$. If Y is compact, then the composed map, $B \circ A$ is closed in x.

Third Composition Lemma: Let A be a point-to point map from X in Y, and B a point-to-set map from Y to Z. If A is continuous in x, and B is closed in $A(x)$. then the composed map $B \circ A$ is closed in x.

D.4 Variational Principles

The variational problem asks for the function $q(t)$ that minimizes a global functional (function of a function), $J(q)$, with fixed boundary conditions, $q(a)$ and $q(b)$, as shown in Figure D.3. Its general form is given by a local functional, $F(t, q, q')$, and an integral or global functional,

$$J(q) = \int_a^b F(t, q, q')dt \ ,$$

where the prime indicates, as usual, the simple derivative with respect to t, that is, $q' = dq/dt$.

Euler-Lagrange Equation

Consider a 'variation' of $q(t)$ given by another curve, $\eta(t)$, satisfying the fixed boundary conditions, $\eta(a) = \eta(b) = 0$,

$$q = q(\epsilon, t) = q(t) + \epsilon\eta(t) \ \text{ and}$$

$$J(\epsilon) = \int_a^b F\left(t, q(\epsilon, t), q'(\epsilon, t)\right) dt \ .$$
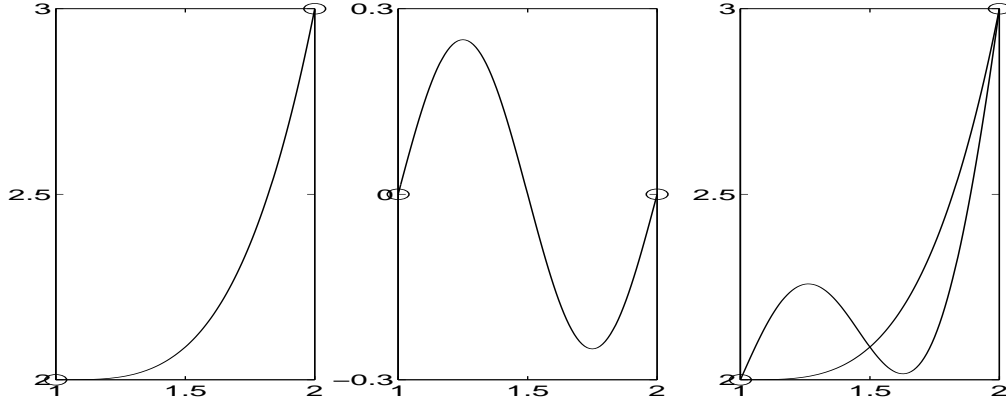
Figure D.3: Variational problem, $q(x)$, $\eta(x)$, $q(x) + \eta(x)$.

A minimizing $q(t)$ must be stationary, that is,

$$\frac{\partial J}{\partial \epsilon} = \frac{\partial}{\partial \epsilon} \int_a^b F\left(t, q(\epsilon, t), q'(\epsilon, t)\right) dt = 0 \; .$$

Since the boundary conditions are fixed, the differential operator affects only the integrand, hence

$$\frac{\partial J}{\partial \epsilon} = \int_a^b \left(\frac{\partial F}{\partial q} \frac{\partial q}{\partial \epsilon} + \frac{\partial F}{\partial q'} \frac{\partial q'}{\partial \epsilon} \right) dt$$

From the definition of $q(\epsilon, t)$ we have

$$\frac{\partial q}{\partial \epsilon} = \eta(t) \; , \quad \frac{\partial q'}{\partial \epsilon} = \eta'(t) \; , \quad \text{hence} \; ,$$

$$\frac{\partial J}{\partial \epsilon} = \int_a^b \left(\frac{\partial F}{\partial q} \eta(t) + \frac{\partial F}{\partial q'} \eta'(t) \right) dt \; .$$

Integrating the second term by parts, we get

$$\int_a^b \frac{\partial F}{\partial q'} \eta'(t) dt = \frac{\partial F}{\partial q'} \eta(t) \Big|_a^b - \int_a^b \frac{d}{dt} \left(\frac{\partial F}{\partial q'} \right) \eta(t) dt \; ,$$

where the first term vanishes, since the extreme points, $\eta(a) = \eta(b) = 0$, are fixed. Hence

$$\frac{\partial J}{\partial \epsilon} = \int_a^b \left(\frac{\partial F}{\partial q} - \frac{d}{dt} \frac{\partial F}{\partial q'} \right) \eta(t) dt \; .$$

Since $\eta(t)$ is arbitrary and the integral must be zero, the parenthesis in the integrand must be zero. This is the Euler-Lagrange equation:

$$\frac{\partial F}{\partial q} - \frac{d}{dt} \frac{\partial F}{\partial q'} = 0 \; .$$

Noether Theorems

Nother theorems establishes very general conditions under which the existence of a symmetry in the system, described by the invariance under the action of a continuous group, implies the existence of a quantity that remains constant in the system's evolution, that is, a conservation law, see for example Byron and Fuller (1969, V-I, Sec. 2.7).

For example, consider a functional $F(t, q, q')$ that does not depends explicitly of q. This situation reveals a symmetry: The system is invariant by a translation on the coordinate q. From Euler-Lagrange equatuion, it follows that the quantity $p = \partial F/\partial q'$ is conserved. In the language of classical mechanics, q would be called a "cyclic coordinate", while p would be called a "generalized moment".

Let us consider the lifeguard's problem from section 5.5. Using the variable t instead of x, and q instead of y, the length of an infinitesimal arch is $ds^2 = dt^2 + dq^2$ and we can build the total travel time using the functional

$$F(t, q, q') = \nu(t)\sqrt{1 + q'}$$

Since the local functional is not a function of q, the Euler-Lagrange equation reduces to $\partial F/\partial q' = K$, where K is a constant. Hence, the lifeguard's problem solution is

$$\nu(t)\frac{q'}{\sqrt{1 + q'}} = K \ .$$

If the resistance index $\nu(t)$ is also independent of t, q' must be a constant, so that q is a straight line, as we have guessed in our very informal solution. In general, the solution to the lifeguard's problem is given by

$$\nu(t)\frac{\tan(\theta)}{\sqrt{1 + \tan(\theta)}} = \nu(t)\sin(\theta) = K \ .$$

Appendix E

Entropy and Asymptotics

"...we can identify that quantity which we commonly designate as (thermodynamic) entropy with the probability of the actual state."

Ludwig Bolttzmann (1844 - 1906).
Wärmetheorie und der Wahrscheinlischkeitrechnung, 1877.

The origins of the entropy concept lay in the fields of Thermodynamics and Statistical Physics, but its applications have extended far and wide to many other phenomena, physical or not. The entropy of a probability distribution, $H(p(x))$, is a measure of uncertainty (or impurity, confusion) in a system whose states, $x \in \mathcal{X}$, have $p(x)$ as probability distribution. We follow closely the presentation in the following references. For the basic concepts: Csiszar (1974), Dugdale (1996), Kinchine (1957) and Renyi (1961, 1970). For MaxEnt characterizations: Gokhale (1975) abd Kapur (1989). For MaxEnt optimization: Censor and Zenios (1994, 1997), Elfving (1980), Fang et al. (1997) and Iusem and Pierro (1987). For posterior asymptotic convergence: Gelman (1995).

For a detailed analysis of the connection between MaxEnt optimization and Bayesian statistics' formalisms, that is, for a deeper view of the relation between MaxEnt and Bayes' rule updates, see Caticha and Giffin (2007) and Caticha (2007).

E.1 Convexity

We first introduce the concept of convexity, that is going to be important throughout this chapter.

Definition: A region $S \in R^n$ is Convex iff, for any two points, $x^1, x^2 \in S$, and weights $0 \leq l_1, l_2 \leq 1 \,|\, l_1 + l_2 = 1$, the convex combination of these two points remains in S, i.e. $l_1 x^1 + l_2 x^2 \in S$.

Theorem Finite Convex Combination: A region $S \in R^n$ is Convex iff any (finite) convex combination of its points remains in the region, i.e., $\forall \quad 0 \leq l \leq 1 \mid 1'l = 1$, $X = [x^1, x^2, \ldots x^m]$, $x^j \in S$,

$$
X\, l = \begin{bmatrix} x_1^1 & x_1^2 & \cdots & x_1^m \\ x_2^1 & x_2^2 & \cdots & x_2^m \\ \vdots & \vdots & \ddots & \vdots \\ x_n^1 & x_n^2 & \cdots & x_n^m \end{bmatrix} \begin{bmatrix} l_1 \\ l_2 \\ \cdots \\ l_m \end{bmatrix} \in S
$$

Proof: By induction in the number of points, m.

Definition: The Epigraph of the function $\varphi : R^n \to R$ is the region of X "above the graph" of φ, i.e.

$$
\mathrm{Epi}\,(\varphi) = \left\{ x \in R^{n+1} \mid x_{n+1} \geq \varphi\left([x_1, x_2, \ldots, x_n]'\right) \right\}
$$

Definition: A function φ is convex iff its epigraph is convex. A function φ is concave iff $-\varphi$ is convex.

Theorem: A differentiable function, $\varphi : R \to R$, with non negative second derivative is convex.

Proof: Consider $x^0 = l_1 x^1 + l_2 x^2$, and the Taylor expansion around x^0,

$$
\varphi(x) = \varphi(x^0) + \varphi'(x^0)(x - x^0) + (1/2)\varphi''(x^*)(x - x^0)^2
$$

where x^* is an appropriate intermediate point. If $\varphi''(x^*) > 0$ the last term is positive. Now, making $x = x^1$ and $x = x^2$ we have, respectively, that $\varphi(x^1) \geq \varphi(x^0) + \varphi'(x^0)l_1(x^1 - x^2)$ and $\varphi(x^2) \geq \varphi(x^0) + \varphi'(x^0)l_2(x^2 - x^1)$ multipying the first inequality by l_1, the second by l_2, and adding them, we obtain the desired result.

Theorem Jensen Inequality: If φ is a convex function,

$$
\mathrm{E}\,(\varphi(x)) \geq \varphi\,(\,\mathrm{E}(X))
$$

For discrete distributions the Jensen inequality is a special case of the finite convex combination theorem. Arguments of Analysis allow us to extend the result to continuous distributions.

E.2   Boltzmann-Gibbs-Shannon Entropy

If $H(p(x))$ is to be a measure of uncertainty, it is reasonable that it should satisfy the following list of requirements. For the sake of simplicity, we present the theory for finite spaces.

1) If the system has n possible states, $x_1, \ldots x_n$, the entropy of the system with a given distribution, $p_i \equiv p(x_i)$, is a function

$$H = H_n(p_1, \ldots, p_n)$$

2) H is a continuous function.

3) H is a function symmetric in its arguments.

4) The entropy is unchanged if an impossible state is added to the system, i.e.,

$$H_n(p_1, \ldots p_n) = H_{n+1}(p_1, \ldots p_n, 0)$$

5) The system's entropy in minimal and null when the system is fully determined, i.e.,

$$H_n(0, \ldots, 0, 1, 0, \ldots 0) = 0$$

6) The system's entropy is maximal when all states are equally probable, i.e.,

$$\frac{1}{n}\mathbf{1} = \arg\max H_n$$

7) A system maximal entropy increases with the number of states, i.e.

$$H_{n+1}\left(\frac{1}{n+1}\mathbf{1}\right) > H_n\left(\frac{1}{n}\mathbf{1}\right)$$

8) Entropy is an extensive quantity, i.e., given two independent systems, with distributions p e q, the entropy of the composite system is additive, i.e.,

$$H_{nm}(r) = H_n(p) + H_m(q) \quad , \quad r_{i,j} = p_i \, q_j$$

The Boltzmann-Gibbs-Shannon measure of entropy,

$$H_n(p) = -I_n(p) = -\sum_{i=1}^{n} p_i \log(p_i) = -\operatorname{E}_i \log(p_i) \quad , \quad 0 \log(0) \equiv 0$$

satisfies requirements (1) to (8), and is the most usual measure of entropy. In Physics it is usual to take the logarithm in Nepper base, while in Computer Science it is usual to take base 2 and in Engineering it is usual to take base 10. The opposite of the entropy, $I(p) = -H(p)$, the Neguentropy, is a measure of Information available about the system.

For the Boltzmann-Gibbs-Shannon entropy we can extend requirement 8, and compute the composite Neguentopy even without independence:

$$
\begin{aligned}
I_{nm}(r) &= \sum_{i=1,j=1}^{n,m} r_{i,j} \log(r_{i,j}) = \sum_{i=1,j=1}^{n,m} p_i \Pr(j \,|\, i) \log\left(p_i \Pr(j \,|\, i)\right) \\
&= \sum_{i=1}^{n} p_i \log(p_i) \sum_{j=1}^{m} \Pr(j \,|\, i) + \sum_{i=1}^{n} p_i \sum_{j=1}^{m} \Pr(j \,|\, i) \log\left(\Pr(j \,|\, i)\right) \\
&= I_n(p) + \sum_{i=1}^{n} p_i \, I_m(q^i) \quad \text{where} \quad q_j^i = \Pr(j \,|\, i)
\end{aligned}
$$

If we add this last identity as item number 9 in the list of requirements, we have a characterization of Boltzmann-Gibbs-Shannon entropy, see Kinchine (1957) and Renyi (1961, 1970).

Like many important concepts, this measure of entropy was discovered and re-discovered several times in different contexts, and sometimes the uniqueness and identity of the concept was not immediately recognized. A well known anecdote refers the answer given by von Neumann, after Shannon asked him how to call a "newly" discovered concept in Information Theory. As reported by Shannon in Tribus and McIrvine (1971, p.180):

"My greatest concern was what to call it. I thought of calling it information, but the word was overly used, so I decided to call it uncertainty. When I discussed it with John von Neumann, he had a better idea. Von Neumann told me, You should call it entropy, for two reasons. In the first place your uncertainty function has been used in statistical mechanics under that name, so it already has a name. In the second place, and more important, nobody knows what entropy really is, so in a debate you will always have the advantage."

E.3   Csiszar's φ-divergence

In order to check that requirement (6) is satisfied, we can use (with $q \propto 1$) the following lemma:

Lemma: Shannon Inequality
If p and q are two distributions over a system with n possible states, and $q_i \neq 0$, then the *Information Divergence* of p relative to q, $I_n(p, q)$, is positive, except if $p = q$, when it is null,

$$I_n(p,q) \equiv \sum_{i=1}^n p_i \, \log\left(\frac{p_i}{q_i}\right) \quad, \quad I_n(p,q) \geq 0 \quad, \quad I_n(p,q) = 0 \Rightarrow p = q$$

Proof: By Jensen inequality, if φ is a convex function,

$$\mathrm{E}\left(\varphi(x)\right) \geq \varphi\left(\mathrm{E}(X)\right)$$

Taking

$$\varphi(t) \;=\; t\ln(t) \;\; \text{and} \;\; t_i \;=\; \frac{p_i}{q_i}$$

$$\mathrm{E}_q(t) \;=\; \sum_{i=1}^n q_i \frac{p_i}{q_i} \;=\; 1$$

$$I_n(p,q) \;=\; \sum q_i \, t_i \log t_i \geq 1 \, \log(1) \;=\; 0$$

Shannon's inequality motivates the use of the Information Divergence as a measure of (non symmetric) "distance" between distributions. In Statistics this measure is known

as the Kullback-Leibler distance. The denominations Directed Divergence or Cross Information are used in Engineering. The proof of Shannon inequality motivates the following generalization of divergence:

Definition: Csiszar's φ-divergence.
Given a convex function φ,

$$d_\varphi(p, q) \;=\; \sum_{i=1}^{n} q_i\, \varphi\left(\frac{p_i}{q_i}\right)$$

$$0\,\varphi\left(\frac{0}{0}\right) \;=\; 0 \;,\quad 0\,\varphi\left(\frac{c}{0}\right) \;=\; c \lim_{t\to\infty} \frac{\varphi(t)}{t}$$

For example, we can define the quadratic and the absolute divergence as

$$\chi^2(p, q) \;=\; \sum \frac{(p_i - q_i)^2}{q_i} \;,\quad \text{for } \varphi(t) \;=\; (t-1)^2$$

$$Ab(p, q) \;=\; \sum \frac{|p_i - q_i|}{q_i} \;,\quad \text{for } \varphi(t) \;=\; |t-1|$$

E.4   Maximum Entropy under Constraints

Given a prior distribution, q, we would like to find a vector p that minimizes the Information Divergence $I_n(p, q)$, where p is under the constraint of being a probability distribution, and maybe also under additional constraints over the expectation of functions taking values on the system's states, that is, we want

$$p^* \in \arg\min I_n(p, q) \;,\; p \geq 0 \mid \mathbf{1}'p = 1 \text{ and } Ap = b \;,\; A\,(m-1) \times n$$

p^* is the *Minimum Information Divergence* distribution, relative to q, given the constraints $\{A, b\}$. We can write the probability normalization constraint as a generic linear constraint, including $\mathbf{1}$ and 1 as the m-th (or 0-th) rows of matrix A and vector b. So doing, we do not need to keep any distinction between the normalization and the other constraints. In this chapter, the operators $\odot$ e $\oslash$ indicate the point (element) wise product and division between matrices of same dimension.

The Lagrangean function of this optimization problem, and its derivatives are:

$$L(p, w) = p' \log(p \oslash q) + w'(b - Ap) \;,$$

$$\frac{\partial L}{\partial p_i} = \log(p_i/q_i) + 1 - w'A^i \;,\quad \frac{\partial L}{\partial w_k} = b_k - A_k p \;.$$

Equating the $n + m$ derivatives to zero, we have a system with $n + m$ unknowns and equations, giving viability and optimality conditions (VOCs) for the problem:

$$p_i \;=\; q_i \exp\left(w'A^i - 1\right) \;\text{ ou }\; p \;=\; q \odot \exp\left((w'A)' - \mathbf{1}\right)$$

$$A_k p \;=\; b_k \;,\; p \geq 0$$

We can further replace the unknown probabilities, p_i, writing the VOCs only on w, the dual variables (Lagrange multipliers),

$$h_k(w) \equiv A_k \left(q \odot \exp \left((w' A)' - \mathbf{1} \right) \right) - b_k = 0$$

The last form of the VOCs motivates the use of iterative algorithms of Gauss-Seidel type, solving the problem by cyclic iteration. In this type of algorithm, one cyclically "fits" one equation of the system, for the current value of the other variables. For a detailed analysis of this type of algorithm, see Censor and Zenios (1994, 1997), Elfving (1980), Garcia et al. (2002) and Iusem and Pierro (1987).

Bregmann Algorithm:

Initialization: Take $t = 0$, $w^t \in R^m$, and

$$p_i^t = q_i \exp \left(w^{t'} A^i - 1 \right)$$

Iteration step: for $t = 1, 2, \ldots$, Take

$$k = (t \bmod m) \quad \text{and} \quad \nu \,|\, \varphi(\nu) = 0 \ , \quad \text{where}$$

$$
\begin{aligned}
w^{t+1} &= \left[w_1^t, \ldots w_{k-1}^t, w_k^t + \nu, w_{k+1}^t, \ldots w_m^t \right]' \\
p_i^{t+1} &= q_i \exp(w^{t+1'} A^i - 1) \ = \ p_i^t \exp(\nu A_k^i) \\
\varphi(\nu) &= A_k p^{t+1} - b_k
\end{aligned}
$$

From our discussion of Entropy optimization under linear constraints, it should be clear that the minimum information divergence distribution for a system under constraints on the expectation of functions taking values on the system's states,

$E_{p(x)} a_k(x) = \int a_k(x) p(x) dx = b_k$, (including the normalization constraint, $a_0 = \mathbf{1}, b_0 = 1$) has the form

$$p(x) = q(x) \exp \left(-\theta_0 - \theta_1 \, a_1(x) - \theta_2 \, a_2(x) \ldots \right)$$

Note that we took $\theta_0 = -(w_0 - 1)$, $\theta_k = -w_k$, and we have also indexed the state i by variable x, so to write the last equation in the standard form used in the statistical literature.

Several distributions commonly used in Statistics can be interpreted as minimum information (or MaxEnt) densities (relative to the uniform distribution, if not otherwise stated) given some constraints over the expected value of state functions. For example:

The Normal distribution is characterized as the distribution of maximum entropy on R^n, given the expected values of its first and second moments, i.e., mean vector and covariance matrix.

The Wishart distribution:

$$f(S \mid \nu, V) \equiv c(\nu, V) \exp \left(\frac{\nu - d - 1}{2} \log(\det(S)) - \sum_{i,j} V_{i,j} S_{i,j} \right)$$

is characterized as the distribution of maximum entropy in the support $S > 0$, given the expected value of the elements and log-determinant of matrix S. That is, writing Γ' for the digamma function,

$$\mathrm{E}(S_{i,j}) = V_{i,j} \quad, \quad \mathrm{E}(\log(\det(S))) = \sum_{k=1}^{d} \Gamma' \left(\frac{\nu - k + 1}{2} \right)$$

The Dirichlet distribution

$$f(x \mid \theta) = c(\theta) \exp \left(\sum_{k=1}^{m} (\theta_k - 1) \log(x_k) \right)$$

is characterized as the distribution of maximum entropy in the support $x \geq 0 \mid \mathbf{1}'x = 1$, given the expected values of the log-coordinates, $\mathrm{E}(\log(x_k))$.

Jeffrey's Rule:

Richard Jeffrey considered the problem of updating an old probability distribution, q, to a new distribution, p, given new constraints on the probabilities of a partition, that is,

$$\sum_{i \in S_k} p_i = \alpha_k \;, \quad \sum_k \alpha_k = 1 \;, \quad S_1 \cup \ldots \cup S_m = \{1, \ldots n\} \;, \quad S_l \cap S_k = \emptyset,\ l \neq k \;.$$

His solution to this problem, known as the *Jeffrey's rule*, coincides with the minimum information divergence distribution, relative to q, given the new constraints. This solution can be expressed analytically as

$$p_i = \alpha_k q_i / \sum_{j \in S_k} q_j \;, \quad k \mid i \in S_k \;.$$

E.5   Fisher's Metric and Jeffreys' Prior

The Fisher Information Matrix, $J(\theta)$, is defined as minus the expected Hessian of the log-likelihood. Under appropriate regularity conditions, the *information geometry* is defined by the metric in the parameter space given by the Fisher information matrix, that is, the geometric lenght of a curve is computed integrating the form $dl^2 = d\theta' J(\theta) d\theta$.

Lemma: The Fisher information matrix can also be written as the covariance matrix of for the gradient of the same likelihood, i.e.,

$$J(\theta) \equiv - \mathrm{E}_{\mathcal{X}} \frac{\partial^2 \log p(x \mid \theta)}{\partial \theta^2} = \mathrm{E}_{\mathcal{X}} \left(\frac{\partial \log p(x \mid \theta)}{\partial \theta} \frac{\partial \log p(x \mid \theta)}{\partial \theta} \right)$$

Proof:

$$\int_{\mathcal{X}} p(x \mid \theta) dx = 1 \Rightarrow \int_{\mathcal{X}} \frac{\partial p(x \mid \theta)}{\partial \theta} dx = 0 \Rightarrow$$

$$\int_{\mathcal{X}} \frac{\partial p(x\,|\,\theta)}{\partial\,\theta} \frac{p(x\,|\,\theta)}{p(x\,|\,\theta)} dx = \frac{\partial \log p(x\,|\,\theta)}{\partial\,\theta} p(x\,|\,\theta) dx = 0$$

differentiating again relative to the parameter,

$$\int_{\mathcal{X}} \left(\frac{\partial^2 \log p(x\,|\,\theta)}{\partial\,\theta^2} p(x\,|\,\theta) + \frac{\partial \log p(x\,|\,\theta)}{\partial\,\theta} \frac{\partial p(x\,|\,\theta)}{\partial\,\theta} \right) dx = 0$$

observing that the second term can be written as

$$\int_{\mathcal{X}} \frac{\partial \log p(x\,|\,\theta)}{\partial\,\theta} \frac{\partial p(x\,|\,\theta)}{\partial\,\theta} \frac{p(x\,|\,\theta)}{p(x\,|\,\theta)} dx = \int_{\mathcal{X}} \frac{\partial \log p(x\,|\,\theta)}{\partial\,\theta} \frac{\partial \log p(x\,|\,\theta)}{\partial\,\theta} p(x\,|\,\theta) dx$$

we obtain the lemma.

Harold Jeffreys used the Fisher metric to define a class of prior distributions, proportional to the determinant of the information matrix,

$$p(\theta) \propto |J(\theta)|^{1/2}.$$

Lemma: Jeffreys' priors are geometric objects in the sense of being invariant by a continuous and differentiable change of coordinates in the parameter space, $\eta = f(\theta)$. The proof follows Zellner (1971, p.41-54):

Proof:

$$J(\theta) = \left[\frac{\partial\,\eta}{\partial\,\theta}\right] J(\eta) \left[\frac{\partial\,\eta}{\partial\,\theta}\right]', \quad \text{hence}$$

$$|J(\theta)|^{1/2} = \left|\frac{\partial\,\eta}{\partial\,\theta}\right| |J(\eta)|^{1/2}, \quad \text{and}$$

$$|J(\theta)|^{1/2}\,d\theta = |J(\eta)|^{1/2}\,d\eta. \quad \text{Q.E.D.}$$

Example: For the multinomial distribution,

$$p(y\,|\,\theta) = n! \prod_{i=1}^{m} \theta_i^{x_i} \Big/ \prod_{i=1}^{m} x_i!\;,\;\; \theta_m = 1 - \sum_{i=1}^{m-1} \theta_i\;,\;\; x_m = n - \sum_{i=1}^{m-1} x_i\;,$$

$$L = \log p(\theta\,|\,x) = \sum_{i=1}^{m} x_i \log \theta_i\;,$$

$$\frac{\partial^2 L}{(\partial\,\theta_i)^2} = -\frac{x_i}{\theta_i^2} + \frac{x_m}{\theta_m^2}\;,\;\;\; \frac{\partial^2 L}{\partial\,\theta_i \partial\,\theta_j} = -\frac{x_m}{\theta_m^2}\;,\;\;\; i,j = 1\ldots m-1\;,$$

$$-\mathrm{E}_{\mathcal{X}} \frac{\partial^2 L}{(\partial\,\theta_i)^2} = \frac{n}{\theta_i} + \frac{n}{\theta_m}\;,\;\;\; -\mathrm{E}_{\mathcal{X}} \frac{\partial^2 L}{\partial\,\theta_i \partial\,\theta_j} = \frac{n}{\theta_m}\;,$$

$$|J(\theta)| = (\theta_1 \theta_2 \ldots \theta_m)^{-1}\;,\;\;\; p(\theta) \propto (\theta_1 \theta_2 \ldots \theta_m)^{-1/2}\;,$$

$$p(\theta\,|\,x) \propto \theta_1^{x_1-1/2} \theta_2^{x_2-1/2} \ldots \theta_m^{x_m-1/2}\;.$$

Hence, in the multinomial exemple, Jeffreys' prior "discounts" half an observation of each kind, while the maxent prior discounts one full observation, and the flat prior discounts none. Similarly, slightly different versions of uninformative priors for the multivariate normal distribution are shown in section C.3. This situation leads to the possible criticism stated in Berger (1993, p.89):

> *"Perhaps the most embarassing feature of noninformative priors, however, is simply that there are often so many of them."*

One response to this this criticism, to which Berger (1993, p.90) explicitly subscribes, is that

> *"it is rare for the choice of a noninformative prior to makedly affect the answer... so that any reasonable noninformative prior can be used. Indeed, if the choice of noninformative prior does have a pronouced effect on the answer, then one is probably in a situation where it is crucial to involve subjective prior information."*

The robustness of the inference procedures to variations on the form of the uninformative prior can tested using sensitivity analysis, as discussed in section A.6. For alternative approaches, on robustness and sensitivity analysis, see Berger (1993, sec.4.7).

In general Jeffrey's priors are not minimally informative in any sense. However, Zellner (1971, p.41-54, Appendix do chapter 2: Prior Distributions Representing "Knowing Little") gives the following argument (attributed to Lindley) to present Jeffreys' priors as asymptotically minimally informative. The information measure of $p(x\,|\,\theta)$, $I(\theta)$; The prior average information, A; The information gain, G, that is, the prior average information associated with an observation, A, minus the prior information measure; and The asymptotic information gain, G_a, are defined as follows:

$$I(\theta) = \int p(x\,|\,\theta)\log p(x\,|\,\theta)dx \; ;$$

$$A = \int I(\theta)p(\theta)d\theta \; ;$$

$$G = A - \int p(\theta)\log p(\theta)d\theta \; ;$$

$$G_a = \int p(\theta)\sqrt{n\,|J(\theta)|}d\theta - \int p(\theta)\log p(\theta)d\theta \; .$$

Although Jeffreys' priors does not in general maximize the information gain, G, the asymptotic convergence results presented in the next section imply that Jeffrey's priors maximize the asymptotic information gain, G_a. For further details and generalizations, see Amari (2007), Amari et al. (1987), Berger and Bernardo (1992), Berger (1993), Bernardo and Smith (2000), Hartigan (1983), Jeffreys (1961), Scholl (1998), and Zhu (1998).

E.6   Posterior Asymptotic Convergence

The Information Divergence, $I(p, q)$, can be used to proof several asymptotic results that are fundamental to Bayesian Statistics. We present in this section two of these basic results, following Gelman (1995, Ap.B).

Theorem Posterior Consistency for Discrete Parameters:

Consider a model where $f(\theta)$ is the prior in a discrete parameter space, $\Theta = \{\theta^1, \theta^2, \ldots\}$, $X = [x^1, \ldots x^n]$ is a series of observations, and the posterior is given by

$$f(\theta^k \mid X) \propto f(\theta^k)\, p(X \mid \theta^k) = f(\theta^k) \prod_{i=1}^{n} p(x^i \mid \theta^k)$$

Further, assume that this model there is a single value for the vector parameter, θ^0, that gives the best approximation for the "true" predictive distribution $g(x)$, in the sense that it minimizes the information divergence

$$\{\theta^0\} \;=\; \arg\min_k I\big(g(x), p(x \mid \theta^k)\big)$$

$$I\big(g(x), p(x \mid \theta^k)\big) \;=\; \int_{\mathcal{X}} g(x) \log\left(\frac{g(x)}{p(x \mid \theta^k)}\right) dx \;=\; \mathrm{E}_{\mathcal{X}} \log\left(\frac{g(x)}{p(x \mid \theta^k)}\right)$$

Then,

$$\lim_{n\to\infty} f(\theta^k \mid X) = \delta(\theta^k, \theta^0)$$

Heuristic Argument: Consider the logarithmic coefficient

$$\log\left(\frac{f(\theta^k \mid X)}{f(\theta^0 \mid X)}\right) \;=\; \log\left(\frac{f(\theta^k)}{f(\theta^0)}\right) + \sum_{i=1}^{n} \log\left(\frac{p(x^i \mid \theta^k)}{p(x^i \mid \theta^0)}\right)$$

The first term is a constant, and the second term is a sum which terms have all negative expected (relative to x, for $k \neq 0$) value since, by our hypotheses, θ^0 is the unique argument that minimizes $I(g(x), p(x \mid \theta^k))$. Hence, (for $k \neq 0$), the right hand side goes to minus infinite as n increases. Therefore, at the left hand side, $f(\theta^k \mid X)$ must go to zero. Since the total probability adds to one, $f(\theta^0 \mid X)$ must go to one, QED.

We can extend this result to continuous parameter spaces, assuming several regularity conditions, like continuity, differentiability, and having the argument θ^0 as a interior point of Θ with the appropriate topology. In such a context, we can state that, given a pre-established small neighborhood around θ^0, like $C(\theta^0, \epsilon)$ the cube of side size ϵ centered at θ^0, this neighborhood concentrates almost all mass of $f(\theta \mid X)$, as the number of observations grows to infinite. Under the same regularity conditions, we also have that Maximum a Posteriori (MAP) estimator is a consistent estimator, i.e., $\widehat{\theta} \to \theta^0$.

The next results show the convergence in distribution of the posterior to a Normal distribution. For that, we need the Fisher information matrix identity from the last section.

Theorem Posterior Normal Approximation:
The posterior distribution converges to a Normal distribution with mean θ^0 and precision $nJ(\theta^0)$.

Proof (heuristic): We only have to write the second order log-posterior Taylor expansion centered at $\widehat{\theta}$,

$$\log f(\theta \,|\, X) \;=\; \log f(\widehat{\theta} \,|\, X) \;+\; \frac{\partial \, \log f(\widehat{\theta} \,|\, X)}{\partial \, \theta}(\theta - \widehat{\theta})$$

$$+\frac{1}{2}(\theta - \widehat{\theta})'\frac{\partial^{\,2} \log f(\widehat{\theta} \,|\, X)}{\partial \, \theta^2}(\theta - \widehat{\theta}) \;+\; \mathcal{O}(\theta - \widehat{\theta})^3$$

The term of order zero is a constant. The linear term is null, for $\widehat{\theta}$ is the MAP estimator at an interior point of Θ. The Hessian in the quadratic term is

$$H(\widehat{\theta}) = \frac{\partial^{\,2} \log f(\widehat{\theta} \,|\, X)}{\partial \, \theta^2} \;=\; \frac{\partial^{\,2} \log f(\widehat{\theta})}{\partial \, \theta^2} + \sum_{i=1}^{n} \frac{\partial^{\,2} \log p(x^i \,|\, \widehat{\theta})}{\partial \, \theta^2}$$

The Hessian is negative definite, by the regularity conditions, and because $\widehat{\theta}$ is the MAP estimator. The first term is constant, and the second is the sum of n i.i.d. random variables. At the other hand we have already shown that the MAP estimator, and also that all the posterior mass concentrates around θ^0. We also see that the Hessian grows (in average) linearly with n, and that the higher order terms can not grow super-linearly. Also for a given n and $\theta \to \widehat{\theta}$, the quadratic term dominates all higher order terms. Hence, the quadratic approximation of the log-posterior in increasingly more precise, Q.E.D.

Given the importance of this result, we present an alternative proof, also giving the reader an alternative way to visualize the convergence process, see Figure 1.

Theorem MLE Normal Approximation:
The Maximum Likelihood Estimator (MLE) is asymptotically Normal, with mean θ^0 and precision $nJ(\theta^0)$.

Proof (schematic): Assuming all needed regularity conditions, from the first order optimality conditions,

$$\frac{1}{n}\sum_{i=1}^{n}\frac{\partial \, \log p(x^i \,|\, \widehat{\theta})}{\partial \, \theta} = 0$$

hence, by the mean value theorem, there is an intermediate point $\widetilde{\theta}$ such that

$$\frac{1}{n}\sum_{i=1}^{n}\frac{\partial \, \log p(x^i \,|\, \theta^0)}{\partial \, \theta} = \frac{1}{n}\sum_{i=1}^{n}\frac{\partial^{\,2} \log p(x^i \,|\, \widetilde{\theta})}{\partial \, \theta^2}(\theta^0 - \widehat{\theta})$$

or, equivalently,

$$\sqrt{n}(\widehat{\theta} - \theta^0) = -\left[\frac{1}{n}\sum_{i=1}^{n}\frac{\partial^{\,2} \log p(x^i \,|\, \widetilde{\theta})}{\partial \, \theta^2}\right]^{-1}\frac{1}{\sqrt{n}}\sum_{i=1}^{n}\frac{\partial \, \log p(x^i \,|\, \theta^0)}{\partial \, \theta}$$

We assume the regularity conditions are enough to assure that

$$-\left[\frac{1}{n}\sum_{i=1}^{n}\frac{\partial^{\,2} \log p(x^i \,|\, \widetilde{\theta})}{\partial \, \theta^2}\right]^{-1} \to J(\theta^0)^{-1}$$

for the MLE is consistent, $\widehat{\theta} \to \theta^0$, and hence so is the mean value point, $\widetilde{\theta} \to \theta^0$; and

$$\frac{1}{\sqrt{n}} \sum_{i=1}^{n} \frac{\partial \log p(x^i \mid \theta^0)}{\partial \theta} \to N(0, J(\theta^0))$$

because we have the sum of n i.i.d. vectors with mean 0 and, by the Information Matrix Identity lemma covariance $J(\theta^0)$.

Hence, we finally have

$$\sqrt{n}(\widehat{\theta} - \theta^0) \to N\left(0, J(\theta^0)^{-1} J(\theta^0) J(\theta^0)^{-1}\right) = N\left(0, J(\theta^0)^{-1}\right)$$

Q.E.D.

Exercises:

1) Implement Bregmann's algorithm. It may be more convenient to number the rows of A from 1 to m, and take $k = (t \bmod m) + 1$.

2) I was given a dice, that I assumed to be honest. A friend of mine lent the dice and reported playing it 60 times, obtaining 4 i's, 8 ii's, 11 iii's, 14 iv's, 13 v's and 10 vi's.
A) What is my Bayesian posterior?
Bi) What was the mean face value? (3.9).
Bii) What is the expected posterior value of this statistic?
C) I called the dice manufacturer, and he told me that this dice is made so that the expected value of this statistic is exactly 4.0. Use Bregmamnn algorithm to obtain the "entropic posterior", that is, the distribution closest to the prior that obeys the given constraints. Use as prior: 1) the uniform; ii) the Bayesian posterior.

3) Discuss the difference between the Bayesian update and the entropic update. What is the information given in each case? Observations or constraints?

4) Discuss the possibility of using the FBST to make hierarchical tests for complex hypotheses using these ideas.

5) Try to give MaxEnt characterizations and Jeffrey's priors for all distributions you know.

Appendix F

Matrix Factorizations

F.1 Matrix Notation

Let us first define some matrix notation. The operator $f:s:t$, to be read *from f to t* with *step s*, indicates the vector $[f, f+s, f+2s, \ldots t]$ or the corresponding index domain. $f:t$ is a short hand for $f:1:t$. The element in the i-th row and j-th column of matrix A is written as $A(i,j)$ or, with subscript row index and superscript column index, as A_i^j. Index vectors can be used to build a matrix by extracting from a larger matrix a given sub-set of rows and columns. For example, $A(1:m/2, n/2:n)$ or $A_{1:m/2}^{n/2:n}$ is the northeast block, i.e. the block with the first rows and last columns, from A. The next example shows a more general case of this notation,

$$
A = \begin{bmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{bmatrix} , \quad r = \begin{bmatrix} 1 & 3 \end{bmatrix} , \quad s = \begin{bmatrix} 3 & 1 & 2 \end{bmatrix} ,
$$

$$
A_r^s = A(r,s) = \begin{bmatrix} 13 & 11 & 12 \\ 33 & 31 & 32 \end{bmatrix} .
$$

The suppression of an index vector indicates that the corresponding index spans all values in its current context. Hence, $A(i, :)$ or A_i indicates the i-th row, and $A(:, j)$ or A^j indicates the j-th column of matrix A.

A single or multiple list of matrices is referenced by one or more indices in braces, like $A\{k\}$ or $A\{p, q\}$. As for element indices, for double lists we may also use the subscript - superscript alternative notation for $A\{p, q\}$, namely, $A\{_p^q\}$. This compact notation is specially usefull for building block matrices, like in the following example,

$$
A = \begin{bmatrix} A\{_1^1\} & A\{_1^2\} & \ldots & A\{_1^s\} \\ A\{_2^1\} & A\{_2^2\} & \ldots & A\{_2^s\} \\ \vdots & \vdots & \ddots & \vdots \\ A\{_r^1\} & A\{_r^2\} & \ldots & A\{_r^s\} \end{bmatrix} .
$$

Hence, $A\{p,q\}(i,j)$ or $A\{{}^q_p\}{}^j_i$ indicates the element in the i-th row and j-th column of the block situated at the p-th block of rows and q-th block of columns of matrix A, $A\{p,q\}(:,j)$ or $A\{{}^q_p\}{}^j$ indicates the j-th column of the same block, and so on.

An upper case letter usually stands for (or starts) a matrix name, while lower case letters are used for vectors or scalars. Whenever recommended by style or tradition, we may slightly abuse the notation using upper case for the name of a matrix and lower case for some of its parts. For example, we may write x^j, instead of X^j for the j-th column of matrix X.

The vectors of zeros and ones, with appropriate dimension given by the context, are $\mathbf{0}$ and $\mathbf{1}$. The transpose of matrix M is M', and the transpose inverse, M^{-t}. In $(M+v)$, where v is a column (row) vector of compatible dimension, v is added to each column (row) of matrix M.

A tilde accent, $\widetilde{A}$, indicates some simple transformation of matrix A. For exemple, it may indicate a row and / or column permutation, see next subsection. A tilde accent may also indicate a normalization, like $\widetilde{x} = (1/||x||)x$.

The p-norm of a vector x is given by $||x||_p = (\sum |x_i|^p)^{-p}$. Hence, for a non-negative vector x, we can write its 1-norm as $||x||_1 = \mathbf{1}'x$. $V > 0$ is a positive definite matrix. The Hadamard or pointwise product, $\odot$, is defined by $M = A \odot B \Leftrightarrow M^j_i = A^j_i B^j_i$. The squared Frobenius norm of a matrix is defined by $\text{frob2}(M) = \sum_{i,j}(M^j_i)^2$.

The Diagonal operator, diag, if applied to a square matrix, extracts the main diagonal as a vector, and if applied to a vector, produces the corresponding diagonal matrix.

$$\text{diag}(A) = \begin{bmatrix} A^1_1 \\ A^2_2 \\ \vdots \\ A^n_n \end{bmatrix}, \quad \text{diag}(a) = \begin{bmatrix} a_1 & 0 & \dots & 0 \\ 0 & a_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & a_n \end{bmatrix}, \quad \text{diag}^2(A) = \begin{bmatrix} A^1_1 & 0 & \dots & 0 \\ 0 & A^2_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & A^n_n \end{bmatrix}.$$

The Kroneker product of two matrices is a block matrix where block $\{i,j\}$ is the second matrix multiplied by element (i,j) of the first matrix:

$$A \otimes B = \begin{bmatrix} A^1_1 B & A^2_1 B & \cdots \\ A^1_2 B & A^2_2 B & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

The following properties are easy to check:

- $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$

- $(A \otimes B)' = A' \otimes B'$

- $(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$

The Vec operator stacks the columns of a matrix into a single column vector, that is, if A is $m \times n$,

$$\text{Vec}(A) = \begin{bmatrix} A^1 \\ \vdots \\ A^n \end{bmatrix}$$

The following properties are easy to ckeck:

- $\text{Vec}(A + B) = \text{Vec}(A) + \text{Vec}(B)$

- $\text{Vec}(AB) = \begin{bmatrix} AB^1 \\ \vdots \\ AB^n \end{bmatrix} = (I \otimes A)\,\text{Vec}(B)$

Permutations and Partitions

We now introduce some concepts and notations related to the permutation and partition of an $m \times n$ matrix A. A permutation matrix is a matrix obtained by permuting rows and columns of the identity matrix, I. To perform on I a given row (column) permutation yields the corresponding row (column) permutation matrix.

Given row and column permutation matrices, P and Q, the corresponding vectors of permuted row and column indices are

$$p = (P \begin{bmatrix} 1 \\ 2 \\ \vdots \\ m \end{bmatrix})'$$

$$q = \begin{bmatrix} 1 & 2 & \dots & n \end{bmatrix} Q$$

To perform a row (column) permutation on a matrix A, obtaining the permuted matrix $\tilde{A}$, is equivalent to multiply it at the left (right) by the corresponding row (column) permutation matrix. Moreover, if p (q) is the corresponding vector of permuted row (column) indices,

$$A_p = PA = I_p A \ , \quad A^q = AQ = I^q \ .$$

Exemple: Given the martices

$$A = \begin{bmatrix} 11 & 12 & 13 \\ 21 & 22 & 23 \\ 31 & 32 & 33 \end{bmatrix} \ , \quad P = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \ , \quad Q = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \ ,$$

$$p = q = \begin{bmatrix} 3 & 1 & 2 \end{bmatrix} , \quad PA = \begin{bmatrix} 31 & 32 & 33 \\ 11 & 12 & 13 \\ 21 & 22 & 23 \end{bmatrix} , \quad AQ = \begin{bmatrix} 13 & 11 & 12 \\ 23 & 21 & 22 \\ 33 & 31 & 32 \end{bmatrix} .$$

A square matrix, A, is *symmetric* iff it is equal to its transpose, that is, iff $A = A'$. A *symmetric permutation* of a square matrix A is a permutation of form $\tilde{A} = PAP'$ or $\tilde{A} = Q'AQ$, where P or Q are (row or column) permutation matrices. A square matrix, A, is *orthogonal* iff its inverse equals its transpose, that is, iff $A^{-1} = A'$. The following statements are easy to check:

(a) A permutation matrix is orthogonal.

(b) A symmetric permutation of a symmetric matrix is still symmetric.

A permutation vector, p, and a termination vector, t, define a partition of m original indices in s classes:

$$\begin{bmatrix} p\,(1) \\ \vdots \\ p\,(t(1)) \end{bmatrix} , \quad \begin{bmatrix} p\,(t(1)+1) \\ \vdots \\ p\,(t(2)) \end{bmatrix} \quad \cdots \quad \begin{bmatrix} p\,(t(s-1)+1) \\ \vdots \\ p\,(t(s)) \end{bmatrix}$$

$$\text{where } t(0) = 0 < t(1) < \ldots < t(s-1) < t(s) = m .$$

We define the corresponding permutation and partition matrices, P and T, as

$$P = I_{p(1\,:\,m)} = \begin{bmatrix} P\{1\} \\ P\{2\} \\ \vdots \\ P\{s\} \end{bmatrix} , \quad P\{r\} = I_{p(t(r-1)+1\,:\,t(r))} ,$$

$$T_r = \mathbf{1}'\,(P\{r\}) \quad \text{and} \quad T = \begin{bmatrix} T_1 \\ \vdots \\ T_s \end{bmatrix} .$$

These matrices facilitate writing functions of a given partition, like

• The indices in class r

$$P\{r\}\,(1\,:\,m) = P\{r\} \begin{bmatrix} 1 \\ \vdots \\ m \end{bmatrix} = \begin{bmatrix} p\,(t(r-1)+1) \\ \vdots \\ p\,(t(r)) \end{bmatrix} ;$$

• The number of indices in class r

$$T_r \mathbf{1} = t(r) - t(r-1) ;$$

- A sub-matrix with the row indices in class r

$$P\{r\} A = \begin{bmatrix} A_{p(t(r-1)+1)} \\ \vdots \\ A_{p(t(r))} \end{bmatrix} \; ;$$

- The summation of the rows of a submatrix with row indices in class r

$$T_r A = \mathbf{1}' \left(P\{r\} A \right) \; ;$$

- The rows of a matrix, added over each class

$$T A = \begin{bmatrix} T_1 A \\ \vdots \\ T_s A \end{bmatrix} \; .$$

Note that a matrix T represents a partition of m idices into s classes if T has dimension $s \times m$, $T_h^j \in \{0,1\}$ and T has orthogonal rows. The element T_h^j indicates if the index $j \in 1:m$ is in class $h \in 1:s$.

F.2 Dense LU, QR and SVD Factorizations

Vector Spaces and Projectors

Given two vectors, $x, y \in R^n$, their *scalar product* is defined as

$$x'y = \sum_{i=1}^{n} x_i y^i \; .$$

With this definition in mind, it is easy to check that the scalar product satisfies the following properties of the *inner product* operator:

1. $< x \mid y >=< y \mid x >$, symmetry.

2. $< \alpha x + \beta y \mid z >= \alpha < x \mid z > +\beta < y \mid z >$, linearity.

3. $< x \mid x >\geq 0$, semi-positivity.

4. $< x \mid x >= 0 \Leftrightarrow x = 0$, positivity.

A given inner product defines the following norm,

$$\|x\| \equiv < x \mid x >^{1/2} \; ;$$

that can in turn be used to define the angle between two vectors:

$$\Theta(x, y) \equiv \arccos(< x \mid y > / \|x\| \|y\|) .$$

Let us consider the linear subspace generated by the columns of a matrix A, m by n, $m \geq n$:

$$C(A) = \{y = Ax, x \in R^n\} .$$

$C(A)$ is called the *image* of A, and the complement of $C(A)$, $N(A)$, is called the *null space* of A,

$$N(A) = \{y \mid A'y = 0\} .$$

The projection of a vector $b \in R^m$ in the column space of A is defined by the relations:

$$y = P_{C(A)}b \leftrightarrow y \in C(A) \wedge (b - y) \perp C(A)$$

or, equivalently,

$$y = P_{C(A)}b \leftrightarrow y = Ax \wedge A'(b - y) = 0 .$$

In the sequel we assume that A has full rank, i.e., that its columns are linearly independent. It is easy to check that the projection of b in $C(A)$ is given by the linear operator

$$P_A = A(A'A)^{-1}A' .$$

If $y = A((A'A)^{-1}A'b)$, then it is obvious that $y \in C(A)$. At the other hand,

$$A'(b - y) = A'(I - A(A'A)^{-1}A')b = (A' - IA')b = 0 .$$

Orthogonal Matrices

A real square matrix Q is said to be *orthogonal* iff its inverse is equal to its transpose, that is, $Q'Q = I$. The columns of an orthogonal matrix Q are a orthonormal basis for R^n. The quadratic norm of a vector v, given by

$$\|v\|^2 \equiv \sum (v_i)^2 = v'v ,$$

is not changed by an orthogonal transform, since

$$(Qv)'(Qv) = v'Q'Qv = v'Iv = v'v .$$

Given a vector in R^2, $\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$, a rotation of this vector by an angle θ is given by the linear transform

$$G\{\theta\}x = \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} .$$

A rotation is an orthogonal transform, since

$$G\{\theta\}'G\{\theta\} = \begin{bmatrix} \cos(\theta)^2 + \sin(\theta)^2 & 0 \\ 0 & \cos(\theta)^2 + \sin(\theta)^2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

The Givens rotation is a linear operator whose matrix is the identity, except for the insertion of a bidimensional rotation matrix:

$$G\{i, j, \theta\} = \begin{bmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & \cos(\theta) & & \sin(\theta) & & \\ & & & \ddots & & & \\ & & -\sin(\theta) & & \cos(\theta) & & \\ & & & & & \ddots & \\ & & & & & & 1 \end{bmatrix}.$$

The left multiplication of matrix A by a Givens transform, $G'A$, rotates rows i and j of A counterclockwise by an angle θ. Since the product of orthogonal transforms is still orthogonal, we can use a sequence of Givens rotations to build more complex orthogonal transforms.

We now define some simple bidimensional rotations that will be used as building blocks in the construction of several algorithms. Let us consider, in R^2, a vector v, a symmetric matrix S, and an asymmetric matrix A,

$$v = \begin{bmatrix} x \\ y \end{bmatrix}, \quad S = \begin{bmatrix} p & q \\ q & r \end{bmatrix}, \quad A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

In order to set to zero the second component of vector v by means of a left rotation, $G\{\theta_v\}' v$, it is possible to use the angle

$$\theta_v = \arctan\left(\frac{y}{x}\right).$$

In order to diagonalize the symmetric matrix by a symmetric rotation, $G\{\theta_{diag}\}' S G\{\theta_{diag}\}$, it is possible to use the angle

$$\theta_{diag} = \frac{1}{2} \arctan\left(\frac{2q}{r - p}\right).$$

In order to symmetrize the asymmetric matrix by means of a left rotation, $G\{\theta_{sym}\}' A$, it is possible to use the angle

$$\theta_{sym} = \arctan\left(\frac{b - c}{a + d}\right).$$

Hence, it is possible to diagonalize the asymmetric matrix by means of a symmetriza-tion followed by a diagonalization operation. Alternatively, it is possible to use the left and right of Jacobi rotations, $J\{\theta_r\}' A J\{\theta_l\}$, defined as follows

$$\theta_{sum} = \theta_r + \theta_l = \arctan\left(\frac{c+b}{d-a}\right) \quad , \quad \theta_{dif} = \theta_r - \theta_l = \arctan\left(\frac{c-b}{d+a}\right) \quad \text{or}$$

$$J\{\theta_r\}' = G\{\theta_{sum}/2\}' G\{-\theta_{dif}/2\}' \quad , \quad J\{\theta_l\} = G\{\theta_{dif}/2\} G\{\theta_{dif}/2\} \ .$$

when computing the rotation matrices, there is no need to make explicit use of the rotation angles, nor is it necessary to use trigonometric functions, but only to compute the factors $c = \sin(\theta)$ and $s = \sin\theta$, directly as

$$c = \frac{x}{\sqrt{x^2+y^2}} \quad , \quad s = \frac{-y}{\sqrt{x^2+y^2}} \ .$$

In order to avoid numerical overflow, one can use the procedure

- Se $y == 0$, then $c = 1$, $s = 0$.

- Se $y \geq x$, then $t = -x/y$, $s = 1/\sqrt{1+t^2}$, $c = st$.

- Se $y < x$, then $t = -y/x$, $c = 1/\sqrt{1+t^2}$, $s = ct$.

QR Factorization

Given a full rank real matrix A, $m \times n$, $m \geq n$, it is always possible to find an orthogonal matrix Q such that $A = Q \begin{bmatrix} R \\ 0 \end{bmatrix}$, where R is a square upper triangular matrix. This is the QR factorization (or decomposition) of matrix A. The orthogonal factor, $Q = [C \mid N]$ gives an orthonormal basis for R^m, where the first n columns give an orthonormal base for $C(A)$, and the last $m - n$ columns give an orthonormal base for $N(A)$, as can be easily checked by the identity $Q'A = \begin{bmatrix} R \\ 0 \end{bmatrix}$. In the sequel a QR factorization algorithm is presented.

The following example illustrates a rotation sequence that takes a 5×3 matrix to upper triangular form. Every index pair, (i, j), indicates a rotation used to zero the position at row i column j. We assume that the original matrix is dense, that is, that the matrix has no zero elements, and illustrate the sparsity pattern in the matrix as the algorithm progresses.

$$(1, 5) * (1, 4)(1, 3)(1, 2) * (2, 5)(2, 4)(2, 3) * (3, 5)(3, 4)*$$

$$
\begin{bmatrix} x & x & x \\ x & x & x \\ x & x & x \\ x & x & x \\ 0 & x & x \end{bmatrix}
\begin{bmatrix} x & x & x \\ 0 & x & x \\ 0 & x & x \\ 0 & x & x \\ 0 & x & x \end{bmatrix}
\begin{bmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \\ 0 & 0 & x \\ 0 & 0 & x \end{bmatrix}
\begin{bmatrix} x & x & x \\ 0 & x & x \\ 0 & 0 & x \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}
$$

Least Squares

Given an over-determined system, $Ax = b$ where A is $m \times n$, $m > n$, vector x^* is a least squares solution to the system iff x^* minimizes the quadratic norm of the residual, that is,

$$ x^* = Arg \min_{x \in R^n} \|Ax - b\| \ , $$

Since an orthogonal rotation does not change the square norm of a vector, one can seek the least square solution to this system minimizing the residual of the system transformed by the orthogonal factor of the QR factorization of A,

$$ \|Q'(Ax - b)\|^2 = \|\begin{bmatrix} R \\ 0 \end{bmatrix} x - \begin{bmatrix} c \\ d \end{bmatrix}\|^2 = \|Rx - c\|^2 + \|0x - d\|^2. $$

From the last expression one can see that the solution and the residual of the original problem are given by

$$ x^* = R^{-1}c \ , \quad y = Ax^* \quad \text{and} \quad z = Q \begin{bmatrix} 0 \\ d \end{bmatrix}. $$

Since the last $m - n$ columns of Q are an orthonormal basis of $N(A)$, we see that $z \perp C(A)$, and can therefore conclude that $y = P_A b$.

LU and Cholesky Factorizations

Given a matrix A, the *elementary operation* given by the *multiplier m_i^j*, is the operation of subtracting from row i the row j multiplied by m_i^j. The elementary operation applied to the identity matrix generates the corresponding *elementary matrix*,

$$
M\{i, j\} = \begin{bmatrix}
1 & & & & & & & \\
& \ddots & & & & & & \\
& & 1 & & & & & \quad j \\
& & \vdots & \ddots & & & & \\
& & -m_i^j & & 1 & & & \quad i \\
& & \vdots & & & \ddots & & \\
& & & & & & 1 &
\end{bmatrix}
$$

Applying a elementary operation to matrix A is equivalent to multiplying A from the left by the corresponding elementary matrix.

In the *Gaussian elimination* algorithm we use a sequence of elementary operations to bring A to upper triangular form,

$$MA = M\{n, n-1\}M\{n-1, n-2\}M\{n, n-2\}\cdots$$

$$M\{3, 2\}\cdots M\{n-1, 2\}M\{n, 2\}M\{2, 1\}\cdots M\{n-1, 1\}M\{n, 1\}A = U \ .$$

Multiplier m_i^j is computed as the current matrix element at position (i, j) divided by the *pivot* element at the diagonal position (j, j). Elementary operation $M\{i, j\}$ is used to *eliminate* (zero) the position (i, j). The elementary operations are performed in an order that prevents the zeros created at previous steps to be filled again.

The next example shows the steps of Gaussian elimination on a small matrix. The multipliers, in italic, are stored at the positions corresponding to the zeros they created.

$$\begin{bmatrix} 2 & 1 & 3 \\ 2 & 3 & 6 \\ 4 & 4 & 6 \end{bmatrix} \quad \rightarrow \quad \begin{bmatrix} 2 & 1 & 3 \\ \mathit{1} & 2 & 3 \\ \mathit{2} & 2 & 0 \end{bmatrix} \quad \rightarrow \quad \begin{bmatrix} 2 & 1 & 3 \\ \mathit{1} & 2 & 3 \\ \mathit{2} & \mathit{1} & -3 \end{bmatrix}$$

The inverse of the product of this sequence of elementary matrices has the lower triangular form, that is,

$$M^{-1} = M^{-1}\{n, 1\}M^{-1}\{n-1, 1\}\cdots M^{-1}\{2, 1\}M^{-1}\{n, 2\}M^{-1}\{n-1, 2\}$$

$$\cdots M^{-1}\{3, 2\}\cdots M^{-1}\{n, n-2\}M^{-1}\{n-1, n-2\}M^{-1}\{n, n-1\} \ .$$

$$L = M^{-1} = \begin{bmatrix} 1 & & & & \\ m_2^1 & 1 & & & \\ \vdots & \vdots & \ddots & & \\ m_{n-1}^1 & m_{n-1}^2 & & 1 & \\ m_n^1 & m_n^2 & \cdots & m_n^{n-1} & 1 \end{bmatrix} \ .$$

Therefore the algorithm finds the LU factorization, $A = LU$. The lower and upper triangular form of L and U allow us to easily compute $L^{-1}z$ and $U^{-1}z$ by simple forward and backward substitution. Hence, $A^{-1}z = U^{-1}(L^{-1}z)$ can be computed in just two substitution steps.

In case we factor a symmetric matrix $V = LU$, we can collect the diagonal elements of U in a diagonal matrix D, and write $V = LDL'$. If S is positive definite we can take the square roots of the diagonal elements and write $D = D^{1/2}D^{1/2}$.

Defining $C = LD^{1/2}$, we have $V = CC'$, the *Cholesky factor* of V. For reasons of numerical stability, it is recommended to take the square roots of each diagonal elements just before we use it as a *pivot element*, and then eliminate the elements of its column, see Pissanetzky (1984).

Quadratic Programming

The *quadratic programming* problem with equality constraints is the minimization of the objective function

$$f(y) \equiv (1/2)y'Wy + c'y \ , \quad W = W'$$

with the constraints

$$g_i(y) \equiv N_i'y = d_i.$$

The gradients of f and g_i are given by

$$\nabla_y f = y'W + c' \ , \ \text{and } \nabla_y g_i = N_i' \ .$$

The Lagrange (first order) optimality conditions state that the constraints are in effect, and that objective function gradient equals a linear combination of gradients of the constraint functions, Hence, the solution may be obtained from the *Lagrange multipliers*, i.e., the vector l with the coefficients of the aformentioned linear combination.

$$N'y = d \ \wedge \ y'W + c' = l'N' \ ,$$

or, in matrix form,

$$\begin{bmatrix} N' & 0 \\ W & N \end{bmatrix} \begin{bmatrix} y \\ l \end{bmatrix} = \begin{bmatrix} d \\ c \end{bmatrix} \ .$$

These equations are known as the *normal system*, with a symmetric coefficient matrix. If quadratic form W is positive definite, i.e. if $\forall x \ x'Wx \geq 0 \ \wedge \ x'Wx = 0 \Leftrightarrow x = 0$, and the constraint matrix N is full rank, the coefficient matrix of the normal system is also positive definite.

SVD Factorization

The SVD factorization takes a real matrix A, $m \times n$, $m \geq n$, to a diagonal matrix, D, by left and right multiplication by orthogonal matrices $D = U'AV$, Let us first consider the case $m = n$, i.e. a square matrix.

The Jacobi algorithm is an iterative procedure that, at each iterations, "concentrates" the matrix in the diagonal by a Jacobi rotation,

$$J\{i,j,\theta_r\}' A\{k\} J\{i,j,\theta_l\} = A\{k+1\} =$$

$$\begin{bmatrix} A\{k+1\}_1^1 & \cdots & A\{k+1\}_1^i & \cdots & A\{k+1\}_1^j & \cdots & A\{k+1\}_1^n \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ A\{k+1\}_i^1 & \cdots & A\{k+1\}_i^i & \cdots & 0 & \cdots & A\{k+1\}_i^n \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ A\{k+1\}_j^1 & \cdots & 0 & \cdots & A\{k+1\}_j^j & \cdots & A\{k+1\}_j^n \\ \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ A\{k+1\}_n^1 & \cdots & A\{k+1\}_n^i & \cdots & A\{k+1\}_n^j & \cdots & A\{k+1\}_n^n \end{bmatrix}$$

Let us consider the sum of squares of of-diagonal elements of A, $\mathrm{Off}_2(A)$. We can see that

$$\mathrm{Off}_2(A\{k{+}1\}) = \mathrm{Off}_2(A\{k\}) - (A\{k\}_i^j)^2 - (A\{k\}_j^i)^2$$

Hence, choosing at each iteration the index pair that maximizes the sum of squares of the corresponding elements, the algorithms converges linearly to a diagonal matrix.

The Jacobi algorithm gives a constructive proof for the existence of the SVD factorization, and is the basis of several efficient numerical algorithms.

If A is a rectangular matrix, one can first find its QR factorization, and then apply Jacobi algorithm to the upper triangular R factor. If A is square and symmetric, the obtained factorization is known as the *eigenvalue decomposition* of A.

The orthogonal matrices U and V can be interpreted as orthonormal bases in the respective m and n dimensional spaces. The values at the diagonal of S are called the *singular values* of matrix A, and can be interpreted geometrically as the scaling factors of the map $A = UDV'$, taking each versor of the basis V to a scaled versor of the basis U.

Complex Matrices

Many techniques developed in this section for real matrices can be generalized to complex matrices. Practical and elegant methods of obtaining and describing such generalizations are the described by Hemkumar (1994) using *Cordic transforms* (COordinate Rotation Digital Computer). Such a transform is applied to a 2×2 complex matrix M in the form of *internal and external rotations pairs*,

$$\begin{bmatrix} c(\phi) & -s(\phi) \\ s(\phi) & c(\phi) \end{bmatrix} \begin{bmatrix} e(i\alpha) & 0 \\ 0 & e(i\beta) \end{bmatrix} \begin{bmatrix} Ae(ia) & Be(ib) \\ Ce(ic) & De(id) \end{bmatrix} \begin{bmatrix} e(i\gamma) & 0 \\ 0 & e(i\delta) \end{bmatrix} \begin{bmatrix} c(\psi) & -s(\psi) \\ s(\psi) & c(\psi) \end{bmatrix}$$

The elegance of these Cordic transforms comes from the following observations: The internal transform affects only the imaginary exponents of the matrix elements, while the external transform can be independently applied to the real and the imaginary parts of the matrix, that is,

$$\begin{bmatrix} e(i\alpha) & 0 \\ 0 & e(i\beta) \end{bmatrix} \begin{bmatrix} Ae(ia) & Be(ib) \\ Ce(ic) & De(id) \end{bmatrix} \begin{bmatrix} e(i\gamma) & 0 \\ 0 & e(i\delta) \end{bmatrix} =$$

$$\begin{bmatrix} Ae(ia') & Be(ib') \\ Ce(ic') & De(id') \end{bmatrix} = \begin{bmatrix} Ae(i(a+\alpha+\gamma)) & Be(i(b+\alpha+\delta)) \\ Ce(i(c+\beta+\gamma)) & De(i(d+\beta+\gamma)) \end{bmatrix}$$

$$\begin{bmatrix} c(\phi) & -s(\phi) \\ s(\phi) & c(\phi) \end{bmatrix} \begin{bmatrix} A_r' + iA_i' & B_r' + iB_i' \\ C_r' + iC_i' & D_r' + iD_i' \end{bmatrix} \begin{bmatrix} c(\psi) & -s(\psi) \\ s(\psi) & c(\psi) \end{bmatrix} =$$

$$\begin{bmatrix} c(\phi) & -s(\phi) \\ s(\phi) & c(\phi) \end{bmatrix} \begin{bmatrix} A_r' & B_r' \\ C_r' & D_r' \end{bmatrix} \begin{bmatrix} c(\psi) & -s(\psi) \\ s(\psi) & c(\psi) \end{bmatrix}$$

$$+i\left(\begin{bmatrix} c(\phi) & -s(\phi) \\ s(\phi) & c(\phi) \end{bmatrix}\begin{bmatrix} A'_i & B'_i \\ C'_i & D'_i \end{bmatrix}\begin{bmatrix} c(\psi) & -s(\psi) \\ s(\psi) & c(\psi) \end{bmatrix}\right)$$

The following table defines some useful internal and external transforms. Type I transforms change the imaginary exponents of the matrix elements at one of the diagonals. Transforms of Type R, C and D make real the elements in a row, column or diagonal.

Type	Value
I_{main}	$\alpha = -\beta = \gamma = -\delta = (d-a)/2$
I_{off}	$\alpha = -\beta = -\gamma = \delta = (c-b)/2$
R_{up}	$\alpha = \beta = -(b+a)/2 \ ; \ \gamma = -\delta = (b-a)/2$
R_{low}	$\alpha = \beta = -(d+c)/2 \ ; \ \gamma = -\delta = (d-c)/2$
C_{left}	$\alpha = -\beta = (c-a)/2 \ ; \ \gamma = \delta = -(c+a)/2$
C_{right}	$\alpha = -\beta = (d-b)/2 \ ; \ \gamma = \delta = -(d+b)/2$
D_{main}	$\alpha = \beta = -(d+a)/2 \ ; \ \gamma = -\delta = (d-a)/2$
D_{off}	$\alpha = \beta = -(b+c)/2 \ ; \ \gamma = -\delta = (b-c)/2$

It is easy to see that a sequence of internal transforms is equivalent to a single internal transform whose parameters are the sum of the coresponding parameters of the transforms in the sequence.

Combining internal and external transforms, it is possible to create HT's for several interesting algorithms. For example, the HT's of type I, II and III in the following table can be used to obtain the SVD factorization of a complex matrix, much like the Jacobi algorithm. A type I transform applies R_{low} followed by a rotation, making the matrix upper triangular. A type II transform applies D_{main}, I_{off} followed by a diagonalization. For Hermitian (self-adjoint) matrices, the diagonalization is obtained using only one transform of type III

Type	Internal	External
I	$\alpha = \beta = -(d+c)/2 \ ; \ \gamma = -\delta = (d-c)/2$	$\phi = 0 \ ; \ \psi = \arctan(C/D)$
II	$\alpha = -(a+b)/2 \ ; \ \beta = \gamma = -\delta = (b-a)/2$	$\phi \pm \psi = \arctan(B/(D \mp A))$
III	$\alpha = -\beta = -\gamma = \delta = -b/2$	$\phi = \psi = \arctan(2B/(D-A))/2$

Exercises

1. Use the fundamental properties of the inner product to prove that:

   (a) The Cauchy-Scwartz inequality: $|<x\,|\,y>| \le \|x\|\|y\|$. Suggestion: Compute $\|x - \alpha y\|^2$ for $\alpha = <x\,|\,y>^2\,/\|y\|$.

   (b) The triangular inequality: $\|x+y\| \le \|x\| + \|y\|$.

(c) In which case do we have equality or strict Cauchy-Schwartz inequality? Relate your answer to the definition of angle between two vectors.

2. Use the definition of inner product in R^n to prove the parallelogram law: $\|x + y\|^2 + \|x - y\|^2 = 2\|x\|^2 + 2\|y\|^2$.

3. A matrix is idempotent, or a non-orthogonal projector, iff $P^2 = P$. Prove that:

   (a) $R = (I - P)$ is idempotent.

   (b) $R^n = C(P) + C(R)$.

   (c) All eigenvalues of P are 0 or $+1$. Suggestion: Show that if 0 is a root of the characteristic polynomial of P, $\varphi_P(\lambda) \equiv \det(P - \lambda I)$, than $(1 - \lambda) = 1$ is a root of $\varphi_R(\lambda)$.

4. Prove that $\forall P$ idempotent and symmetric, $P = P_{C(P)}$. Suggestion: Show that $P'(I - P) = 0$.

5. Prove that the projection operator into a given vector subspace, V, P_V, is unique and symmetric.

6. Prove Pythagoras theorem: $\forall b \in R^m, u \in V$ we have $\|b - u\|^2 = \|b - P_V b\|^2 + \|P_V b - u\|^2$.

7. Assume we have the QR factorization of a matrix A. Consider a new matrix, $\tilde{A}$, obtained from A by the substitution of a single column. How could we update our orthogonal factorization using only $3n$ rotations? Suggestion: (a) Remove the altered column of A and update the factorization using at most n rotations. (b) Rotated by the new column by the current orthogonal factor. $\tilde{a} = Q'a = R^{-t}A'a$. (c) Add $\tilde{a}$ as the last column of $\tilde{A}$, and update the factorization using $2n$ rotations.

8. Compute the LDL and Cholesky factorizations of matrix

$$
\begin{bmatrix}
4 & 12 & 8 & 12 \\
12 & 37 & 29 & 38 \\
8 & 29 & 45 & 50 \\
12 & 38 & 50 & 113
\end{bmatrix}.
$$

9. Prove that:

   (a) $(AB)' = B'A'$.

   (b) $(AB)^{-1} = B^{-1}A^{-1}$.

   (c) $A^{-t} \equiv (A^{-1})' = (A')^{-1}$.

10. Describe four algorithms to compute $L^{-1}x$ and $L^{-t}x$, accessing the unit diagonal and lower triangular matrix L row by row or column by column.

F.3 Sparse Factorizations

As indicated in chapter 4, we present in this appendix some aspects related to the sparse factorization. This material has strong connections with the issues discussed in chapter 4, but is more mathematical in its nature, and can be omitted by the reader interested mostly in the purely epistemological aspects of decoupling.

Computing the Cholesky factorization of a $n \times n$ matrix involves on the order of n^3 arithmetical operations. Large models may have thousands of variables, so it seems that decoupling large models requires a lot of work. Nevertheless, in practice, matrices appearing in large models are typically sparse and structured. A matrix is called *sparse* if it has many zero elements, otherwise it is called *dense*. A sparse matrix is called *structured* if its non-zero-elements (NZEs) are arranged in a "nice" pattern. As we will see in the next sections, we may be able to obtain a Cholesky factor, L, of a (permuted) sparse and structured matrix V, that 'preserves' some of its sparsity and structure, hence decreasing the computational work.

F.3.1 Sparsity and Graphs

In the discussion of sparsity and structure, the language of graph theory is very helpful. This section gives a quick review of some of the basic concepts on directed and undirected graphs, and also defines the process of vertex elimination.

A Directed Graph, or DG, $\mathcal{G} = (\mathcal{V}, \mathcal{A})$ has a set of vertices or nodes, $\mathcal{V}$, indexed by natural numbers, and a set or directed arcs, $\mathcal{A}$, where each arc joins two vertices. We say that arc $(i, j) \in \mathcal{A}$ goes from node i to node j. When drawing a graphical representation of a DG, it is usual to represent vertices by dots, and arcs by a arrows between the dots. In a DG, we say that i is a parent of j, $i \in pa(j)$, or that j is a child of i, $j \in ch(i)$, if there is an arc going from i to j. The children of i, the children of its children, and so on, are the descendents of i. If j is a descendent of i we say that there is a *path* in $\mathcal{G}$ going from i to j. A *cycle* is a path from a given vertex to itself. An arch from a vertex to itself, (j, j) is called a *loop*. In some situations we spare the effort of multiple definitions of essentially the same objects by referring to the same graph with or without all possible loops.

There is yet another representation for a DG, $\mathcal{G}$, given by $(\mathcal{V}, B)$, where the *adjacency matrix*, B, is the Boolean matrix $B(i, j) = 1$ if arc $(i, j) \in \mathcal{A}$, and 0 otherwise. The key element relating the topics presented in this and the previous section, is the Boolean matrix B indicating the non-zero elements of the numerical matrix A, $B_i^j = I(A_i^j \neq 0)$. In this way, the graph $\mathcal{G} = (\mathcal{V}, B)$ is used to represent the sparsity pattern of a numerical matrix A.

A Directed Acyclic Graph, DAG, has no cycles. A *separator* $S \subset \mathcal{V}$ separates i from

j if any path from i to j goes through a vertex in S. A vertex j is a *spouse* of vertex i, $j \in f(i)$, if they have a child in common. A *tree* is a DAG where each vertex has exactly one parent, except for the root vertex, that has no parent. The leafs of a tree are the vertices with no children. A graph composed by several trees is a *forest*.

An Undirected Graph, or UG, is a DG where, if arc (i, j) is in the graph, so is its opposite, (j, i). An UG can also be represented as $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, where each undirected edge, $\{i, j\} \in \mathcal{E}$, stands for the pair of opposite directed arcs, (i, j) and (j, i). Obviously, the adjacency matrix of a UG is a symmetric matrix, and vice-versa.

$$
\begin{array}{ccccccccccc}
1 & & 3 & \to & 5 & & 1 & & 3 & - & 5 & & & & 3 & & \\
\downarrow & \nearrow & & & \searrow & , & | & / & | & & \backslash & , & & & & & \\
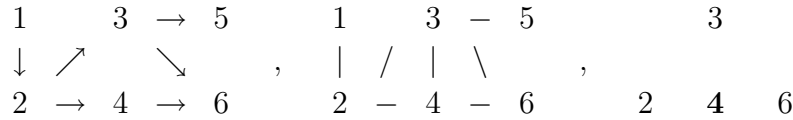2 & \to & 4 & \to & 6 & & 2 & - & 4 & - & 6 & & 2 & & 4 & & 6
\end{array}
$$

Figure 2: A DAG and its Moral Graph.

The moral graph of the DAG $\mathcal{G}$, $\mathcal{M}(\mathcal{G})$, is the undirected graph with the same nodes as $\mathcal{G}$, and edges joining nodes i and j if they are immediate relatives in $\mathcal{G}$. The immediate relatives of a node in $\mathcal{G}$ include its parents, children and spouses (but not brooders or sisters). The set of immediate relatives of i is also called the Markov blanket of i, $\overline{m}(i)$, hence, $j \in \overline{m}(i)$ if j is a neighbor of i in the moral graph. Figure 2 represents a DAG, its moral graph, and the Markov blanket of one of its vertices.

Sometimes it is important to consider an order on the vertex set, established by an 'index vector' q, in (a subset of) $\mathcal{V} = \{1, 2, \ldots N\}$. For example, we can consider the natural order $q = [1, 2, \ldots N]$, or the order given by a permutation, $q = [q(1), q(2), \ldots q(N)]$.

In order not to make language and notation too heavy, we may refer to the vertex 'set' q, meaning the set of elements in vector q. Also, given two index vectors, $a = [a(1), \ldots a(A)]$ and $b = [b(1), \ldots b(B)]$, the index vector $c = a \cup b$, has all the indices in a or b. Similarly, $c = a \backslash b$ has all the indices in a that are not in b. These are essentially set operations but, since an index vector also establishes an order of its elements, $c = [c(1), \ldots c(C)]$, this order, if not otherwise indicated, has somehow to be chosen.

We define the elimination process in the UG, $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, $\mathcal{V} = \{1, \ldots N\}$ given an elimination order, $q = [q(1), \ldots q(N)]$, as the sequence of *elimination graphs* $\mathcal{G}_k = (\mathcal{V}_k, \mathcal{E}_k)$ where, for $k = 1 \ldots n$,

$$
\mathcal{V}_k = \{q(k), q(k+1), \ldots q(n)\}, \quad \mathcal{E}_1 = \mathcal{E}, \quad \text{and, for } k > 1 ,
$$

$$
\{i, j\} \in \mathcal{E}_k \iff \begin{cases} \{i, j\} \in \mathcal{E}_{k-1} , \text{ or} \\ \{q(k-1), i\} \in \mathcal{E}_{k-1} \text{ and } \{q(k-1), j\} \in \mathcal{E}_{k-1} . \end{cases}
$$

that is, when eliminating vertex $q(k)$, we make its neighbors a *clique*, adding all missing edges between them.

The *filled graph* is the graph $(\mathcal{V}, \mathcal{F})$, where $\mathcal{F} = \cup_{k=1}^n \mathcal{E}_k$. The original edges and the filled edges in $\mathcal{F}$ are, respectively, the edges in $\mathcal{E}$ and in $\mathcal{F} \backslash \mathcal{E}$.

Figure 3 shows a graph with 6 vertices, the elimination graphs, and the filled graph, considering the elimination order $q = [1, 3, 6, 2, 4, 5]$.

```
1  −  3            3                                  1  −  3
|  ×     \      /  | \   2  −  6   2            4     |  ×  |  \
2     6  |   2  −  6  |     ×  |   |  \         |     2  −  6  |
   /     /      /     /  5     4   5  −  4      5     |  ×  |  /
5     4      5     4                                  5  −  4
```
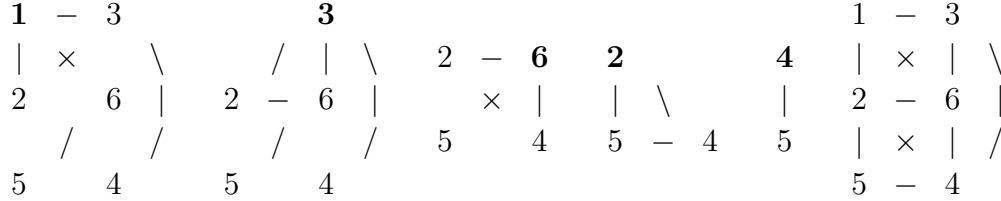
Figure 3: Elimination Graphs.

There is a computationally more efficient form of obtaining the filled graph, known as *simplified elimination*: In the simplified version of the elimination graphs, $\mathcal{G}_k^*$, when eliminating vertex $q(k)$, we add only the clique edges incident to its neighbor, $q(l)$, that is next in the elimination order. Figure 4 shows the simplified elimination graphs and the filled graph corresponding to the elimination process in Figure 3; The vertex being eliminated is in boldface, and his next (in the elimination order) neighbor in italic.

```
1  −  3            3                                  1  −  3
|  ×     \      /  | \   2  −  6   2            4     |  ×  |  \
2     6  |   2     6  |     /  |   |  \         |     2  −  6  |
   /     /      /     /  5     4   5     4      5     |  ×  |  /
5     4      5     4                                  5  −  4
```
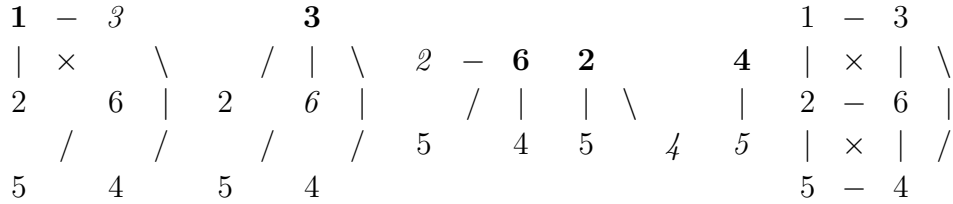
Figure 4: Simplified Elimination Graphs.

An elimination order is perfect if it generates no fill. Perfect elimination is the key to relate the vertex elimination process to the theory of chordal graphs, see Stern (1994). Chordal graph theory provides a unified framework for similar elimination processes in several other contexts, see Golumbic (1980) Stern (1994) and Lauritzen (2006). Nevertheless, we will not explore this connection any further in this paper.

The material presented in this section will be used in the next two sections for the analysis of the sparsity structure in Cholesky factorization and Bayesian networks. This structure is the key for efficient decoupling, allowing the computation of large models, used in the analysis of large systems. These structural aspects have been an area of intense research by the designers of efficient numerical algorithms. However, the same area has not been able to attract so much interest in statistical modeling. From the epistemological considerations in the following chapters, we hope to convince the reader that this is a topic

that deserves to receive much more attention from the statistical modeler.

F.3.2 Sparse Cholesky Factorization

Let us begin with some matrix notation. Given a matrix A, and index vectors p and q, the equivalent notations $A(p,q)$ or A_p^q indicate the (sub) matrix of rows and columns extracted from A according to the indices in p and q. In particular, if p and q have single indices, i and j, $A(i,j)$ or A_i^j indicate the element of A in row i and column j. The next example shows a more general case:

$$
p = \begin{bmatrix} 2 \\ 3 \\ 1 \end{bmatrix} , \quad q = \begin{bmatrix} 3 \\ 2 \end{bmatrix} , \quad A = \begin{bmatrix} 11 & 12 & 13 \\ 21 & 22 & 13 \\ 31 & 32 & 33 \end{bmatrix} , \quad A_p^q = \begin{bmatrix} 23 & 22 \\ 33 & 32 \\ 13 & 12 \end{bmatrix} .
$$

If $q = [q(1), \ldots q(N)]$ is a permutation of $[1, \ldots N]$, and I is the identity matrix, $Q = I_q$ and $Q' = I^q$ are the corresponding row and column permutation matrices. Moreover, if A a $N \times N$ matrix, $A_q = QA$ and $A^q = AQ'$. The symmetric permutation of A in order q is $A(q,q) = QAQ'$.

Let us consider the covariance structure model of section 3. If we write the variables of the model in a permuted order, q, the new covariance matrix is $V(q,q)$. The statistical model is of course the same, but the Cholesky factor of the two matrices may have a quite a different sparsity structure.

Figure 5 shows the positions filled in the Cholesky factorization of a matrix A, and in the Cholesky factorization of two symmetric permutation of the same matrix, $A(q,q)$. Initial Non Zero Elements, NZEs, are represented by x, initial zeros filled during the factorization are represented by 0, and initial zeros left unfilled are represented by blank spaces.

$$
\begin{array}{c}
1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6
\end{array}
\begin{bmatrix}
1 & x & x & & & x \\
x & 2 & x & & & 0 \\
x & x & 3 & x & & 0 \\
 & & x & 4 & & 0 \\
 & & & & 5 & x \\
x & 0 & 0 & 0 & x & 6
\end{bmatrix}
\begin{bmatrix}
1 & x & x & x & & \\
x & 3 & 0 & x & x & \\
x & 0 & 6 & 0 & 0 & x \\
x & x & 0 & 2 & 0 & 0 \\
 & x & 0 & 0 & 4 & 0 \\
 & x & 0 & 0 & 5 &
\end{bmatrix}
\begin{bmatrix}
5 & & & & x & \\
 & 4 & & & & x \\
 & & 2 & & x & x \\
x & & & 6 & & x \\
 & x & x & & 3 & x \\
 & & x & x & x & 1
\end{bmatrix}
$$

Figure 5: Filled Positions in Cholesky Factorization.

The next lemma connects the numerical elimination process in the Cholesky factorization of a symmetric matrix A, to the vertex elimination process in the UG having as adjacency matrix, B, the sparsity pattern of A.

Elimination Lemma: When eliminating the j-th column in the Cholesky factorization of matrix $A(q, q) = LL'$, we fill the positions in L corresponding to the filled edges in $\mathcal{F}$ at the elimination of vertex $q(j)$.

Given a matrix A, $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, an elimination order q, and the respective filled graph, let us consider the set of row indices of NZE's in L^j, the $j - th$ column of the Cholesky factor, $L \mid QAQ' = LL'$:

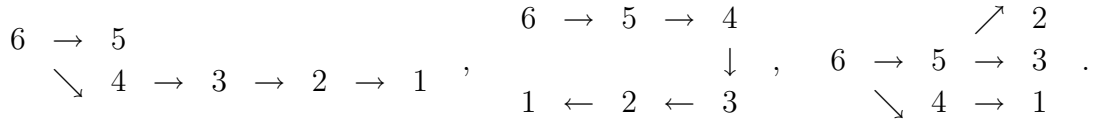$$\mathrm{nze}(L^j) = \{i \mid i > j \wedge \{q(i), q(j)\} \in \mathcal{F}\} + \{j\} \ .$$

$$
\begin{array}{l}
6 \ \rightarrow \ 5 \\
 \ \searrow \ 4 \ \rightarrow \ 3 \ \rightarrow \ 2 \ \rightarrow \ 1
\end{array}
\ ,
\qquad
\begin{array}{l}
6 \ \rightarrow \ 5 \ \rightarrow \ 4 \\
 \ \downarrow \\
1 \ \leftarrow \ 2 \ \leftarrow \ 3
\end{array}
\ ,
\qquad
\begin{array}{l}
 \ \nearrow \ 2 \\
6 \ \rightarrow \ 5 \ \rightarrow \ 3 \\
 \ \searrow \ 4 \ \rightarrow \ 1
\end{array}
\ .
$$

Figure 6: Elimination Trees.

We define the *elimination tree*, $\mathcal{H}$, by

$$
h(j) = \left\{
\begin{array}{ll}
j, & \text{if } \mathrm{nze}(L^j) = \{j\}, \text{ or} \\
\min\{i > j \mid i \in \mathrm{nze}(L^j)\} \ , & \text{otherwise} \ .
\end{array}
\right.
$$

where $h(j)$, the parent of j in $\mathcal{H}$, is the first (non diagonal) NZE in column j of L. Figure 6 shows the elimination trees corresponding to the examples in Figure 5.

Elimination Tree Theorem: For any row index i bellow the diagonal in column j of L, j is a descendant of i in the elimination tree, that is, for any $i > j \mid i \in \mathrm{nze}(L^j)$, the is a path in $\mathcal{H}$ going from i to j.

Proof (see Figure 7): If $i = h(j)$, the result is trivial. Otherwise, (see Figure 7), let $k = h(j)$. But $L_i^j \neq 0 \wedge L_k^j \neq 0 \Rightarrow L_i^k \neq 0$, because $\{q(j), q(i)\}, \{q(j), q(k)\} \in \mathcal{E}_j \Rightarrow \{q(k), q(i)\} \in \mathcal{E}_{j+1}$. Now, either $i = h(k)$, or, applying the argument recursively, we trace a branch of $\mathcal{H}$ $(i, l, \ldots k, j)$, $i > l > \ldots > k > j$. QED.

$$
\begin{array}{l}
1 \\
\quad \ddots \\
\qquad j \\
\qquad \vdots \;\; \ddots \\
\qquad x \;\; \dots \;\; k \\
\qquad\qquad\qquad \ddots \\
\qquad\qquad\qquad\qquad l \\
\qquad\qquad\qquad\qquad \vdots \;\; \ddots \\
\bullet \qquad \bullet \qquad x \;\; \dots \;\; i \\
\qquad\qquad\qquad\qquad\qquad \ddots \\
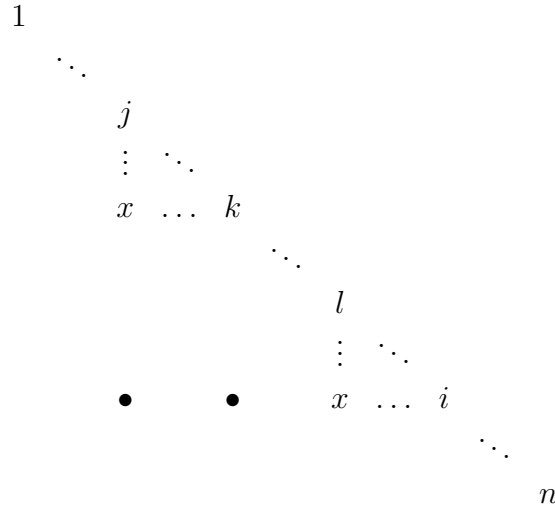\qquad\qquad\qquad\qquad\qquad\qquad n
\end{array}
$$

Figure 7: A Branch in the Elimination Tree.

From the proof of the last theorem we see that the elimination tree portrays the dependencies among the columns for the numeric factorization process. More exactly, we can eliminate column j of A. i.e. compute all the multipliers in column j, M^j, and update all the elements affected by these multipliers, if and only if we have already eliminated all the descendents of j in the elimination tree.

If we are able to perform parallel computations, we can simultaneously eliminate all the columns at a given level of the elimination tree, beginning with the leaves, and finishing at the root. Example 4 considers the elimination of a matrix with the same sparsity pattern of the last permutation in example 1. Its elimination tree is the last one presented at Figure 6. This elimination tree has three levels that, from the leaves to the root, are: $\{1, 3, 2\}$, $\{4, 5\}$, e $\{6\}$.

Hence, we can perform a Cholesky factorization with this sparsity pattern in only 2 steps, as illustrated in the following numerical example:

$$
\begin{bmatrix}
\mathbf{1} & & & 7 & & \\
& \mathbf{2} & & & 8 & \\
& & \mathbf{3} & & 6 & 9 \\
7 & & & 53 & & 2 \\
& 8 & 6 & & 49 & 23 \\
& & 9 & 2 & 23 & 39
\end{bmatrix}
\begin{bmatrix}
1 & & & 7 & & \\
& 2 & & & 8 & \\
& & 3 & & 6 & 9 \\
\mathit{7} & & & \mathbf{4} & & 2 \\
& \mathit{4} & \mathit{2} & & \mathbf{5} & 5 \\
& & \mathit{3} & 2 & 5 & 12
\end{bmatrix}
\begin{bmatrix}
1 & & & 7 & & \\
& 2 & & & 8 & \\
& & 3 & & 6 & 9 \\
\mathit{7} & & & 4 & & 2 \\
& \mathit{4} & \mathit{2} & & 5 & 5 \\
& & \mathit{3} & \frac{1}{2} & 1 & \mathbf{6}
\end{bmatrix}
$$

The sparse matrix literature has many heuristics designed for finding good elimination orders. The example in Figures 8 and 9 show a good elimination order for a 13×13 sparse matrix.

```
 1      3  x
 2      x  8           x
 3            1     x                       x  x
 4               10  x                    x
 5      x  x  x  9                        0
 6                   12           x          x
 7                      13        x
 8                         2  x  x
 9                         x  7  0
10                   x  x  x  0  6        0
11                                  11     x
12      x  x  0                        4  0
13      x     0  x              0  x  0  5
```
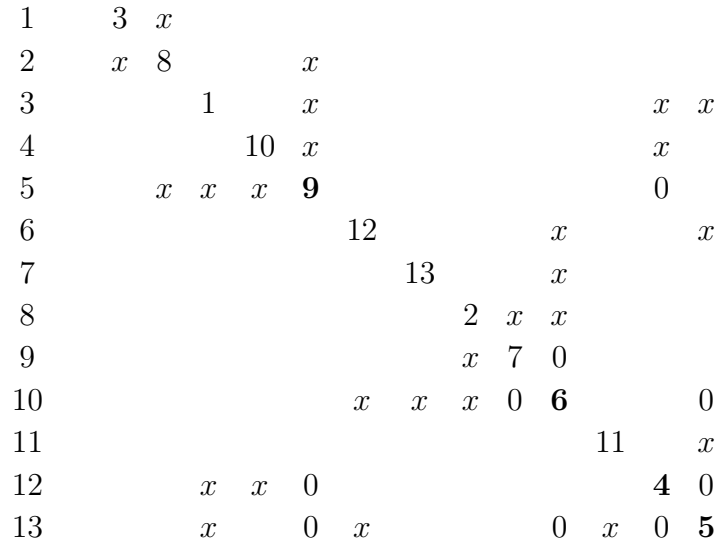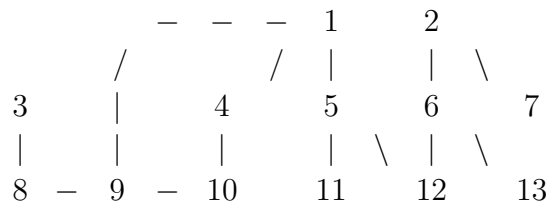
Figure 8: Gibbs Heuristic's Elimination Order.

The elimination order in Figure 8 was found using the Gibbs heuristic, described in Stern (1994, ch.6) or Pissanetzky (1984, ch.x). The intuitive idea of Gibbs heuristic, see Figure 9, is as follows: 1- Starting from a 'peripheral' vertex, in our example, vertex 3; 2- Grow a breath-first tree $\mathcal{T}$ in $\mathcal{G}$. Notice that the vertices at a given level, l, of $\mathcal{T}$ form a separator, S_l, in the graph $\mathcal{G}$. 3- Chose a separator, S_l, that is 'small', i.e. with few vertices, and 'central', i.e. dividing $\mathcal{G}$ in 'balanced' components. 4- Place in q, first the indices of each component separated by S_l, and, at last, the vertices in S_l. 5- Proceed recursively, separating each large component into smaller ones. In our example, we first use separator $S_5 = \{4, 5\}$, dividing $\mathcal{G}$ in three components, $C_1 = \{3, 8, 1, 10, 9\}$ $C_2 = \{12, 13, 2, 7, 6\}$ $C_3 = \{11\}$. Next, we use separators $S_3 = \{9\}$ in C_1, and $S_7 = \{6\}$ in C_2.

The main goal of the techniques studied in this and the last section is to find an elimination order filling as few positions as possible in the Cholesky factor. Once the elimination order has been chosen, simplified elimination can be used to prepare in advance all the data structures holding the sparse matices, hence separating the symbolic (combinatorial) and numerical steps of the factorization. This separation is important in the production of high performance computer programs.
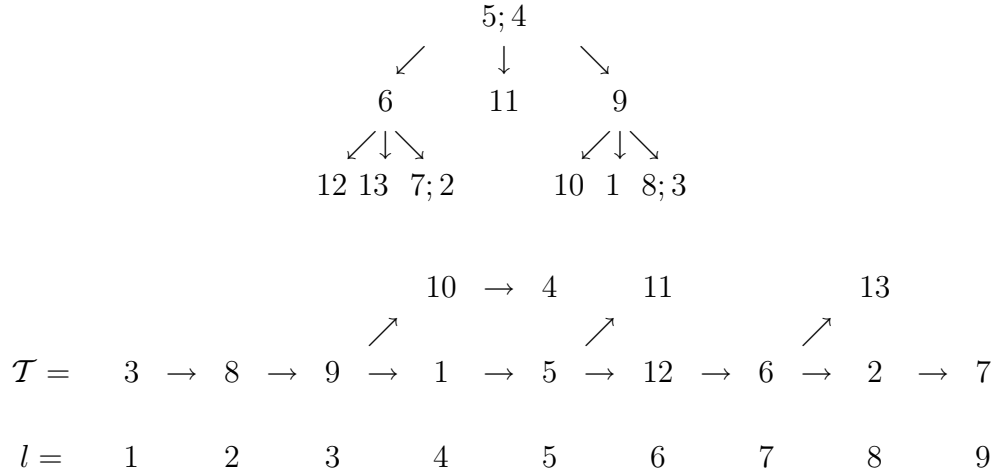
```
              −  −  −  1      2
           /           / |    | \
    3      |      4    5    6    7
    |      |      |    | \  | \
    8  −  9  −  10     11   12   13
```

$$
\begin{array}{ccc}
 & 5;4 & \\
\swarrow & \downarrow & \searrow \\
6 & 11 & 9 \\
\swarrow\downarrow\searrow & & \swarrow\downarrow\searrow \\
12\;13\;\;7;2 & & 10\;\;1\;\;8;3
\end{array}
$$

$$
\mathcal{T} = \quad
\begin{array}{ccccccccccccccc}
 & & & & 10 & \to & 4 & & 11 & & & & 13 \\
 & & & & & \nearrow & & & & \nearrow & & & & \nearrow \\
3 & \to & 8 & \to & 9 & \to & 1 & \to & 5 & \to & 12 & \to & 6 & \to & 2 & \to & 7
\end{array}
$$

$$
l = \quad 1 \qquad 2 \qquad 3 \qquad 4 \qquad 5 \qquad 6 \qquad 7 \qquad 8 \qquad 9
$$

Figure 9: Nested Dissection by Gibbs Heuristic.

F.4 Bayesian Networks

The objective of this section is to show that the sparsity techniques described in the last two section can be applied, almost immediately, to an other important statistical model, namely, Bayesian networks. The presentation in this section follows very closely Cozman (2000). A Bayesian network is represented by a DAG. Each node, i, represents a random variable, x_i. Using the notation established in section 9, we write $i \in n$, where n is the index vector $n = [1, 2, \ldots N]$. The DAG representing the Bayesian network has an arc from node i to node j if the probability distribution of variable x_j is directly dependent on variable x_i.

In many statistical models that arc is interpreted as a direct influence or causal effect of x_i on x_j. Technically, we assume that the joint distribution of the vector x is given in the following product form.

$$
p(x) = \prod_{j \in n} p\left(x_j \mid x_{pa(j)}\right) \ .
$$

The important property of Markov blankets in a Bayesian network is that, given the variables in its Markov blanket, a variable x_i is conditionally independent of any other variable, x_j, in the network, that is, the Markov blanket of a variable 'decouples' this variable from the rest of the network,

$$
p(x_i \mid x_{\overline{m}(i)}, x_j) = p(x_i \mid x_{\overline{m}(i)}) \ .
$$

Inference in Bayesian networks is based on queries, where the distribution of some 'query' variables, x_q, $q = [q(1), \ldots q(Q)]$, is computed, given the observed values of some

'evidence' variables, x_e, $e = [e(1), \ldots e(E)]$. Such queries are performed eliminating, that is marginalizing, integrating, or summing out, all the remaining variables, x_s, that is,

$$p(x_q \,|\, x_e) = \sum_{x_s} p(x) = \sum_{x_s} \prod_{j \in r} p\left(x_j \,|\, x_{pa(j)}\right) \ .$$

We place the indices of the variables to be eliminated in the elimination index vector, $s = r \backslash (q \cup e)$. For now, let us consider the 'requisite' index vector, r, as being just a permutation (reordering) of the original indices in the network, that is, $r = [r(1), \ldots r(R)]$, $R = N$. The 'elimination order' or 'elimination sequence', $s = [s(1), \ldots s(S)]$, will play an important role in what follows.

Let us mention two technical points: First, not all variables of the original network may be needed for a given query. If so, the indices of the unnecessary ones can be removed from the requisite index vector, and the query is performed involving only a proper subset of the original variables, hence, $R < N$. For example, if the network has disconnected components, all the vertices in components having no query variables are unnecessary. Second, the normalization constant of distributions that appear in intermediate computations are costly to obtain and, more important, not needed. Hence, we can perform this intermediate computations with un-normalized distributions, also called 'potentials'.

Making explicit use of the elimination order, $s = [s(1), \ldots s(S)]$, we can write the last equation as

$$p(x_q \,|\, x_e) = \sum_{x_{s(S)}} \cdots \sum_{x_{s(1)}} p(x_{r(1)} \,|\, x_{pa(r(1))}) \times \ldots \times p(x_{r(R)} \,|\, x_{pa(r(R))}) \ .$$

Because $x_{s(1)}$ can only appear in densities $p(x_j \,|\, x_{pa(j)})$ for $j = s(1)$ or $j \in ch(s(1))$, we can separate the first summation, writing

$$p(x_q \,|\, x_e) = \sum_{x_{s(S)}} \cdots \sum_{x_{s(2)}} \left(\prod_{j \in r \backslash (ch(s(1)) \cup s(1))} p(x_j \,|\, x_{pa(j)}) \right)$$

$$\times \left(\sum_{x_{s(1)}} \prod_{j \in ch(s(1)) \cup s(1)} p(x_j \,|\, x_{pa(j)}) \right) \ .$$

Eliminating, i.e. integrating out, the first variable in the elimination order, $x_{s(1)}$, we create a new (joint) potential of the children of the eliminated variable, given its parents and spouses, that is,

$$p(x_{ch(s(1))} \,|\, x_{pa(s(1))}, x_{f(s(1))}) = \sum_{x_{s(1)}} \prod_{j \in ch(s(1)) \cup s(1)} p(x_j \,|\, x_{pa(j)})$$

Next we eliminate $x_{s(2)}$, that is, we collect all potentials containing $x_{s(2)}$, form their joint product, and marginalize on $x_{s(2)}$. We proceed in the elimination order eliminating $x_{s(3)}, x_{s(4)} \ldots x_{s(S)}$, at which point the normalized potentials left give us the distribution $p(x_q \,|\, x_e)$.

We refer to the variables appearing in a joint potential as that potential's cluster. Forming a joint potential is a computation of a complexity that is exponential in the size of its cluster. Hence, it is vital to chose an elimination order that keeps the cluster sizes as small as possible. But the clusters formed in the elimination process of a BN correspond to the cliques appearing in the elimination graphs, as defined in the last two sections. Hence all techniques and heuristics used for finding a good elimination order for Cholesky factorization can be used to obtain a good elimination order for querying a BN. Also, all the abstract combinatorial structures appearing in sparse Cholesky factorization, like elimination trees, have their analogues for computation in BNs. Cozman (2000) develops the complete theory of BNs in a very simple and intuitive way, a way that naturally highlights this analogy. Other authors have already commented on the similarities between several graph decomposition algorithms, see for example Lauritzen (2006, Lecture 4, Probability propagation and related algorithms) for a very general and abstract, but highly mathematical overview.

Appendix G

Monte Carlo Miscellanea

Monte Carlo or, if necessary, Markov Chain Monte Carlo, is the basic tool we use for numerical integration. There are several excellent books on the subject. Hammersley and Handscomb (1964) is a short and intuitive introduction, including some important topics not usually covered at this level, like pseudo-random and quasi-random generators, importance sampling and other variance reduction techniques, and the solution of linear systems. This book is now out of print, but has the advantage of being freely available for download at the internet. Ripley (1987) is an other excellent text covering this material that is still in print. Gilks et al. (1996) gives several excellent and up-to-date review papers on areas that are of interest for statistical modeling. There is a vast literature on MC and MCMC written by physicists. It contains many original, interesting and useful ideas, but sometimes it employs a terminology that is unfamiliar to statisticians. The article of Meng and Wong (1996) can help to overcone this gap.

G.1   Pseudo, Quasi and Subjective Randomness

The implementation of Monte Carlo methods, as described in the following sections, requires a random number generator of i.i.d (independent and identically distributed) random variables uniformly distributed in the unit interval, $[0, 1[$. From this basic uniform generator one gets a uniform generator in the d-dimensional unit box, $[0, 1[^d$ and, from there, non-linear generators for many other multivariate distributions.

Random and Pseudo-Random Generators

The concept of randomness is usually applied to a variable (to be) generated or observed process involving some uncertainty, as in the definition presented by Hammersley and Handscomb (1964, p.10):

> "A random event is an event which has a chance of happening, and probability is a numerical measure of that chance."

Monte Carlo, and several other applications, require a random number generator. With the last definition in mind, engineering devices based on sophisticated physical processes have been built in the hope of offering a source of "true" random numbers. However, these special devices were cumbersome, expensive, not portable nor universally available, and often unreliable. Moreover, practitioners soon realized that simple deterministic sequences could successfully be used to emulate a random generator, as stated in the following quotes (our emphasis) by Hammersley and Handscomb (1964, p.26) and Ripley (1987, p.15):

> "For electronic digital computer it is most convenient to calculate a sequence of numbers one at a time as required, by a completely specified rule which is, however, so devised that no **reasonable** statistical test will detect any significant departure from randomness. Such a sequence is called pseudo-random. The great advantage of a specified rule is that the sequence can be exactly reproduced for purposes of computational checking."

> "A sequence of pseudorandom numbers (U_i) is a deterministic sequence of numbers in $[0, 1]$ having the same **relevant** statistical properties as a sequence of random numbers."

Many deterministic random emulators used today are Linear Congruential Pseudo-Random Generators (LCPRG), as in the following example:

$$x_{i+1} = (ax_i + c) \mod m \; ,$$

where the multiplier a, the increment c and the modulus m should obey the conditions: (i) c and m are relatively prime; (ii) $a - 1$ is divisible by all prime factors of m; (iii) $a - 1$ is a multiple of 4 if m is a multiple of 4. LCPRG's are fast and easy to implement if m is taken as the computer's word range, 2^s, where s is the computer's word size, typically $s = 32$ or $s = 64$. The LCPRG's starting point, x_0, is called the seed. Given the same seed the LCPG will reproduce the same sequence, what is very important for tracing, debugging and verifying application programs.

However, LCPRG's are not an universal solution. For example, it is trivial to devise some statistics that will be far from random, see Marsaglia (1968). There the importance of the words **reasonable** and **relevant** in the last quotations becomes clear: For most Monte Carlo applications these statistics are irrelevant. LCPRG's can also exhibit very long range auto-correlations and, unfortunately, these are more likely to affect long simulated time series required in some special applications. The composition of several

LCPRG's by periodic seed refresh may mitigate some of these difficulties, see Pereira and Stern (1999b). LCPRG's are also not appropriate to some special applications in cryptography, see Boyar (1989). Current state of the art generators are given in Matsumoto and Kurita (1992,1994) and Matsumoto and Nishimura (1998).

Chance is Lumpy - Quasi-Random Generators

"Chance is Lumpy" is Robert Abelson's First Law of Statistics, see Abelson (1995, p.xv). The probabilistic expectation is a linear operator, that is, $E(Ax + b) = AE(x) + b$, where x in random vector and A and b are a determined matrix and vector. The Covariance operator is defined as $\text{Cov}(x) = E((x - E(x)) \otimes (x - E(x)))$. Hence, $\text{Cov}(Ax + b) = A\text{Cov}(x)A'$. Therefore, given n i.i.d. scalar variables, $x_i \,|\, \text{Var}(x_i) = \sigma^2$, the variance of their mean, $m = (1/n)\mathbf{1}'x$, is given by

$$\frac{1}{n}\mathbf{1}' \operatorname{diag}(\sigma^2\mathbf{1}) \frac{1}{n}\mathbf{1} \;=\; \begin{bmatrix} \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{bmatrix} \begin{bmatrix} \sigma^2 & 0 & \cdots & 0 \\ 0 & \sigma^2 & \cdots 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma^2 \end{bmatrix} \begin{bmatrix} \frac{1}{n} \\ \frac{1}{n} \\ \vdots \\ \frac{1}{n} \end{bmatrix} \;=\; \sigma^2/n \ .$$

Hence, the mean's standard deviation is $\text{std}(m) = \sigma/\sqrt{(n)}$. So, mean values of iid random variables converge to their expected values at a rate of $1/\sqrt{(n)}$.

Quasi-random sequences are deterministic sequences built not to emulate random sequences, as pseudo-random sequences do, but to achieve faster convergence rates. For d-dimensional quasi-random sequences, an appropriate measure of fluctuation, called discrepancy, only grows at a rate of $\log(n)^d$, hence growing much slower than $\sqrt{(n)}$. Therefore, the convergence rate corresponding to quasi-random sequences, $\log(n)^d/n$, is much faster than the one corresponding to (pseudo) random sequences, $\sqrt{(n)}/n$. Figure 1 allows the visual comparison of typical (pseudo) random (left) and quasi-random (right) sequences in $[0, 1[^2$. By visual inspection we see that the points of the quasi-random sequence are more "homogeneously scattered" that is, they do not "clump together", as the point of the (pseudo) random sequence often do.

Let us consider an axis-parallel rectangles in the unit box,

$$R = [a_1, b_1[\times [a_2, b_2[\times \ldots [a_d, b_d[\subseteq [0, 1[^2 \ .$$

The discrepancy of the sequence $s_{1:n}$ in box R, and the overall discrepancy of the sequence are defined as

$$D(s_{1:n}, R) = n\text{Vol}(R) - |s_{1:n} \cap R| \ , \quad D(s_{1:n}) = \sup_{R \in [0,1[^d} |D(s_{1:n}, R)| \ .$$

It is possible to prove that the discrepancy of the Halton-Hammersley sequence, defined next, is of order $O(\log(n)^{d-1})$, see Matoušek (1991, ch.2).

Halton-Hammersley sets: Given $d-1$ distinct prime numbers, $p(1), p(2), \ldots p(d-1)$, the i-th point, x^i, in the Halton-Hammersley set, $\{x^1, x^2, \ldots x^n\}$, is

$$x^i = \left[i/n, r_{p(1)}(i), r_{p(2)}(i), \ldots r_{p(d-1)}(i)\right]' , \quad \text{for } i = 1 : n-1 \text{ , where}$$

$$i = a_0 + p(k)a_1 + p(k)^2 a_2 + p(k)^3 a_3 + \ldots , \quad r_{p(k)}(1) = \frac{a_0}{p(k)} + \frac{a_1}{p(k)^2} + \frac{a_2}{p(k)^3} + \ldots .$$

That is, the $(k+1)$-th coordinate of x^i, $x^i_{k+1} = r_{p(k)}(i)$, is obtained by the bit reversal of i written in $p(k)$-ary or base $p(k)$ notation.

The Halton-Hammersley set is a generalization of van der Corput set, built in the bidimensional unit square, $d = 2$, using the first prime number, $p = 2$. The following example, from Hammersley (1964, p.33) and Günther and Jüngel (2003, p.117) builds the 8-point van der Corput set, expressed in binary and decimal notation.

```
function x= corput(n,b)
% size n base b v.d.corput set
m=floor(log(n)/log(b));
u=1:n;  D=[];
for i=0:m
  d= rem(u,b);
  u= (u-d)/b;
  D= [D; d];
end
x=((1./b').^(1:(m\ma1)))*D;
```

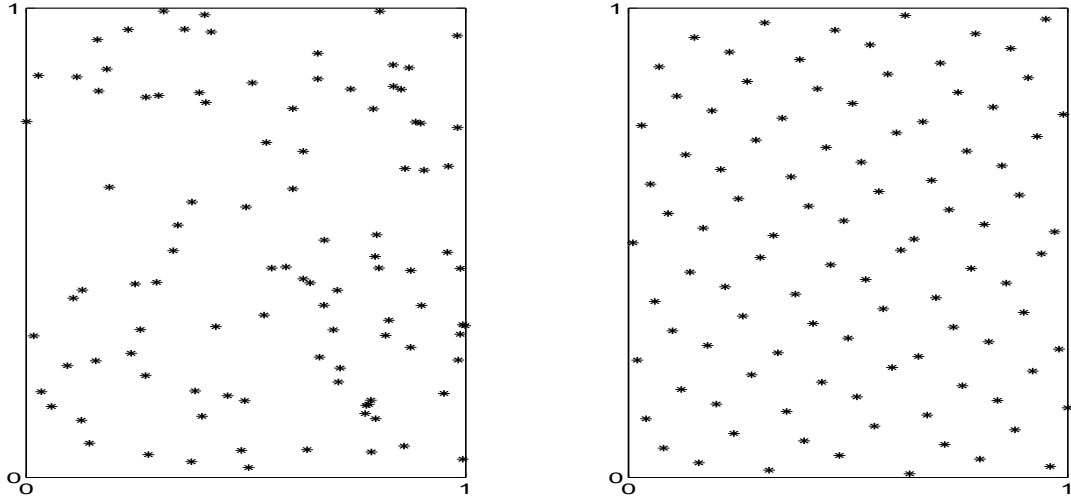| Decimal		Binary	
i	$r_2(i)$	i	$r_2(i)$
1	0.5	1	0.1
2	0.21	10	0.01
3	0.75	11	0.11
4	0.125	100	0.001
5	0.625	101	0.101
6	0.375	110	0.011
7	0.875	111	0.111
8	0.0625	1000	0.0001

Figure G.1: (Pseudo)-random and quasi-random point sets on the unit box

Quasi-random sequences, also known as low-discrepancy sequences, can substitute pseudo-random sequences in some applications of Monte Carlo methods, achieving higher

accuracy with less computational effort, see Merkel (2005), Ökten (1999) and Sen, Samanta and Reese (2006). Nevertheless, since by design the points of a quasi-random sequence tend to avoid each other, strong (negative) correlations are expected to appear. In this way, the very reason that can make quasi-random sequences so helpful, can ultimately impose some limits to their applicability. Some of these problems are commented by Morokoff (1998, p.766):

> *"First, quasi-Monte Carlo methods are valid for integration problems, but may not be directly applicable to simulations, due to the correlations between the points of a quasi-random sequence. ... A second limitation: the improved accuracy of quasi-Monte Carlo methods is generally lost for problems of high dimension or problems in which the integrand is not smooth."*

Subjective Randomness and its Paradoxes

When asked to look at patterns like those in Figure 1, many subjects perceive the quasi-random set as "more random" than the (pseudo) random set. How can this paradox be explained? This was the topic of many psychological studies in the field of subjective randomness. The quotation in the next paragraph is from one of these studies, namely, Falk and Konold (1997, p.306, emphasis are ours):

> *"One major source of confusion is the fact that randomness involves two distinct ideas:* **process** *and* **pattern** *(Zabell, 1992). It is natural to think of randomness as a process that generates unpredictable outcomes (stochastic process according to Gell'Mann, 1994). Randomness of a* **process** *refers to the* **unpredictability** *of the individual event in the series (Lopes, 1982). This is what Spencer Brown (1957) calls* **primary randomness***. However, one usually determines the randomness of the process by means of its output, which is supposed to be* **patternless***. This kind of randomness refers, by definition, to a sequence. It is labeled* **secondary randomness** *by Spencer Brown. It requires that all symbol types, as well as all ordered pairs (diagrams), ordered triplets (trigrams)... n-grams in the sequence be equiprobable. This definition could be valid for any n only in infinite sequences, and it may be approximated in finite sequences only up to ns much smaller than the sequence's length. The entropy measure of randomness (Attneave, 1959, chaps. 1 and 2) is based on this definition.*
>
> *These two aspects of randomness are closely related. We ordinarily expect outcomes generated by a random process to be patternless. Most of them are. Conversely, a sequence whose order is random supports the hypothesis that it was generated by a random mechanism, whereas sequences whose order is not random cast doubt on the random nature of the generating process."*

Spencer-Brown was intrigued by the apparent incompatibility of the notions of primary and secondary randomness. The apparent collision of these two notions generates several interesting paradoxes, taking Spencer-Brown to question the applicability of the concept of randomness to probability and statistical analysis, see Spencer-Brown (1953, 1957) and Flew (1959), Good (1958) and Mundle (1959). See also Henning (2006), Kaptchuk and Kerr (2004), Utts (1991), and Wassermann (1955). In fact, several subsequent psychological studies were able to confirm that, for many subjects, the intuitive or common-sense perception of primary and secondary randomness are quite discrepant. However, a careful mathematical analysis makes it possible to reconcile the two notions of randomness. These are the topics discussed in this section.

The relation between the joint and conditional entropy for a pair of random variables, see appendix E.2,

$$H(i, j) = H(j) + H(i \,|\, j) = H(i) + H(j \,|\, i) \;,$$

motivates the definition of first, second and higher order entropies, defined over the distribution of words of size m in a string of letters from an alphabet of size a.

$$H_1 = \sum_j p(j) \log p(j) \;, \quad H_2 = \sum_{i,j} p(i)p(j \,|\, i) \log p(j \,|\, i) \;,$$

$$H_3 = \sum_{i,j,k} p(i)p(j \,|\, i)p(k \,|\, i, j) \log p(k \,|\, i, j) \;\ldots$$

It is possible to use these entropy measures to access the disorder or lack of pattern in a given finite sequence, using the empirical probability distributions of single letters, pairs, triplets, etc. However, in order to have a significant empirical distribution of m-plets any possible m-plet must be well represented in the sequence, that is, the word size, m, is required to be very short, relative to the sequence log-size, $m << \log_a(n)$.

In the article of Falk and Knold (1997), Figure 2 displays the typical perceived or apparent randomness of Boolean (0-1) bit sequences or black-and-white pixel grids versus the second order entropy of the same strings and grids, see also Attneave (1959). Clearly, there is a remarkable bias of the apparent randomness relative to the entropic measure.

> " *When people invent superfluous explanations because they perceive patterns in random phenomena, they commit what is known in statistical parlance as Type I error The other way of going awry, known as Type H error, occurs when one dismisses stimuli showing some regularity as random. The numerous randomization studies in which participants generated too many alternations and viewed this output as random, as well as the judgments of overalternating sets as maximally random in the perception studies, were all instances of type II error in research results.*" Falk and Konold (1997, p.303).
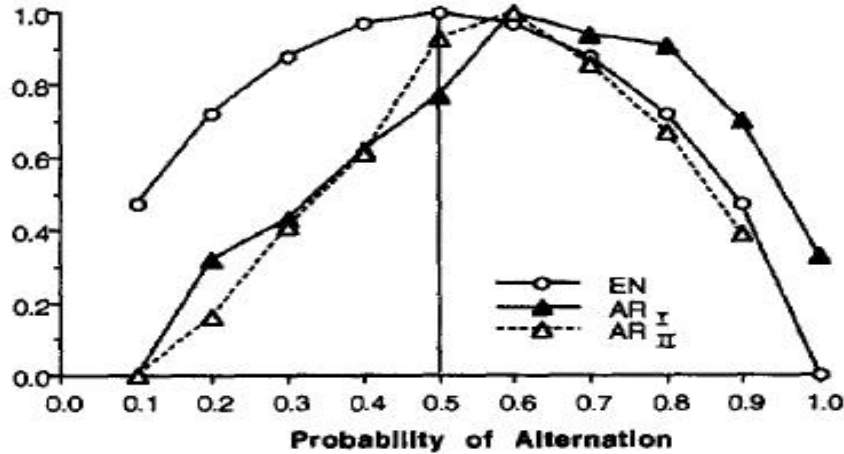
Figure 2: EN, H_2-entropy vs. AR, apparent randomness.

This effect is also known as the *gambler's fallacy* when betting on *cool spots*, expecting the random sequence to "compensate" finite average fluctuations from expected values. Of course, some gamblers exhibit the opposite behavior, preferring to bet on *hot spots*, expecting the same fluctuations to reoccur. These effects are the consequence of a perceived coupling, by a negative or positive correlation or other measure of association, between non overlapping segments that are in fact supposed to be decoupled, uncorrelated or have no association, that is, to be Markovian. For a statistical analysis, see Bonassi et al. (2008). A possible psychological explanation of the gambler's fallacy is given by the constructivist theory of Jean Piaget, see Piaget and Inhelder (1951), in which any "lump" in the sequence is (miss) perceived as non-random order:

> "In analogy to Piaget's operations, which are conceived as internalized actions, perceived randomness might emerge from hypothetical action, that is, from a thought experiment in which one describes, predicts, or abbreviates the sequence. The harder the task in such a thought experiment, the more random the sequence is judged to be." Falk and Konold (1997, p.316).

The same hierarchical decomposition scheme used for higher order conditional entropy measures can be adapted to measure the disorder or patternless of a sequence, relative to a given subject's model of "computer" or generation mechanism. In the case of a discrete string, this generation model could be, for example, a deterministic or probabilistic Turing machine, a fixed or variable length Markov chain, etc. It is assumed that the model is regulated by a code, program or vector parameter, θ, and outputs a data vector or observed string, x. The hierarchical complexity measure of such a model emulates the Bayesian prior and conditional likelihood decomposition, $H(p(\theta, x)) = H(p(\theta)) + H(p(x \mid \theta))$, that is, the total complexity is given by the complexity of the program plus the complexity of the output given the program. This is the starting point for several complexity models,

like Andrey Kolmogorov, Ray Solomonoff and Gregory Chaitin's computational comlexity models, Jorma Rissanen's Minimum Description Length (MDL), and Chris Wallace and David Boulton's Minimum Message Length (MML). All these alternative complexity models can also be used to successfully reconcile the notions of primary and secondary randomness, showing that they are asymptotically equivalent, see Chaitin (1975, 1988), Kac (1983), Kolmogorov (1965), Martin-Löf(1966, 1969).

G.2   Integration and Variance Reduction

This section presents the derivation of generic Monte Carlo procedures for numerical integration. We follow the presentation of Hammersley (1964). Let us consider the integration of a bounded function, $0 \leq f(x) \leq 1$ in the unit interval, $x \in [0, 1]$. The *crud Monte Carlo* unbiased estimate of this integral is the mean value of the function evaluated at uniformly distributed iid random points, $x_i \in [0, 1]$, $i = 1 : n$, with variance

$$\gamma = \int_0^1 f(x)dx \ , \quad \widehat{\gamma}_c = \frac{1}{n}\sum_1^n f(x_i) \ , \quad \sigma_c^2 = \frac{1}{n}\int_0^1 (f(x) - \gamma)^2 \, dx \ .$$

An alternative unbiased estimator is the *hit-or-miss Monte Carlo*, defined by the auxiliary hit indicator function, h,

$$h(x, y) = I(f(x) \geq y) \ , \quad \gamma = \int_0^1\int_0^1 h(x, y)dxdy \ , \quad \widehat{\gamma}_h = \frac{1}{n}\sum_1^n h(x_i, y_i) = \frac{n^*}{n} \ .$$

The variance of this method is that of a Bernoulli variate. Simple manipulation shows that

$$\sigma_h^2 = \frac{\gamma(1 - \gamma)}{n} \ , \quad \sigma_h^2 - \sigma_c^2 = \frac{1}{n}\int_0^1 f(x)(1 - f(x))dx > 0 \ .$$

Hence, hit-or-miss MC is worst than crude MC, as one could guess from the fact that it is using far less information about f at any given point, x_i.

An other alternative is *importance sampling* MC, defined by an auxiliary *sampling distribution*, g, in the integration interval,

$$\gamma = \int f(x)dx = \int \frac{f(x)}{g(x)}g(x)dx = \int \frac{f(x)}{g(x)}dG(x) \ ,$$

$$\widehat{\gamma}_s = \frac{1}{n}\sum_1^n \frac{f(x_i)}{g(x_i)} \ , \quad x_i \sim g \ , \ i = 1 : n \ ; \quad \sigma_s^2 = \frac{1}{n}\int \left(\frac{f(x)}{g(x)} - \gamma\right)^2 dG(x) \ .$$

The importance sampling method can be used on an arbitrary integration interval, as long as we know how to draw the points x_i according to the sampling distribution. The variance of this method is minimized if $g \propto f$, that is if the sampling distribution is

(approximately) proportional to the integrand. In order to achieve a small variance and numerical stability, it is important to keep the sampling ratio bounded, $f/g \leq c$. In particular, if the integration interval is unbounded, the tails of the sampling distribution should "cover" the tails of the integrand.

The formula for σ_s^2 suggests yet another strategy of variance reduction. Let $\varphi(x)$ be a function that closely emulates or mimics $f(x)$, but is easy to integrate analytically (or even numerically). Such a $\varphi(x)$ is known as a *control variate* for $f(x)$. The desired integral can be computed as

$$\gamma = \int \varphi(x)dx + \int (f(x) - \varphi(x))dx = \gamma' + \int (f(x) - \varphi(x))dx .$$

Consider the following estimators and variances,

$$\widehat{\gamma} = \frac{1}{n}\sum_1^n f(x_i) , \quad \widehat{\gamma}' = \frac{1}{n}\sum_1^n \varphi(x_i) ,$$

$$\mathrm{Var}(\widehat{\gamma} - \widehat{\gamma}') = \mathrm{Var}(\widehat{\gamma}) + \mathrm{Var}(\widehat{\gamma}') - 2\mathrm{Cov}\,(\widehat{\gamma}, \widehat{\gamma}') .$$

That is, this the method is useful if the integration and the control variates are strongly (positively) correlated.

Non-Uniform Random Generators

This section considers some elementary methods for producing i.i.d. non-uniform variates, x_i, from a source of uniform variates in the unit interval, $u_i \sim U_{]0,1[}$. Perhaps the simplest example is to produce a Bernoulli variate:

(a) If $0 \leq u_i \leq p$, then $x_i = 1$, else $(p < u_i \leq 1)$, $x_i = 0$.

If $F(x)$ is the cumulative distribution of $f(x)$, and $x_i \sim f$, then $u = F(x_i) \sim U_{[0,1]}$. Hence, if $F(x)$ is invertible, we can just take $x_i = F^{-1}(u_i)$ as a mechanism for generating f distributed variates. For example:

(b) The exponential distribution with mean $1/\lambda$ is given by $f(t) = \lambda \exp(-\lambda t)$, and $F(t) = 1 - \exp(-\lambda t)$. Hence, $t = (-1/\lambda)\ln(u)$ produces an exponential variate.

(c) The Cauchy distribution with location and scale parameters, a, b, is given by $1/f(x) = \pi b(1 + ((x - a)/b)^2)$, $F(x) = (1/2) + (1/\pi)\arctan((x - a)/b)$. Hence, $x = a + b\tan(\pi(u - (1/2)))$ produces the corresponding Cauchy variate.

The characterizations of a distribution in terms of a second distribution may offer an implicit generation mechanism. For example:

(d) The Chi-squared distribution with 2 degrees of freedom, χ_2^2, is a particular case of the exponential with mean $(1/\lambda) = 2$. Hence, $x = -2\ln(u)$ generates a χ_2^2 variate.

(e) A χ_d^2 variate is characterized as a sum of squares of d normal variates. Hence, if d is even, we can generate a χ_d^2 variate as $x = -2\ln(u_1 u_2 \ldots u_{d/2})$.

(f) Counting consecutive λ-exponential arrivals until the threshold $t_1 + t_2 \ldots + t_k \geq 1$ produces a rate-λ Poisson variate, $f(k) = \exp(-\lambda)\lambda^k/k!$.

(g) Appendix B presents characterizations of many discrete distributions by the Poisson, hence providing implicit generation mechanisms for those distributions.

(h) The following two dimensional transformation method generates two i.i.d. standard Normal variates, see Ripley (1987).

$$u, v \sim U_{[0,1]} \ , \quad \theta = 2\pi u \ , \quad r = \sqrt{-2\ln(v)} \ , \quad x = r\cos(\theta) \ , \quad y = r\sin(\theta) \ .$$

To check the method consider the transformation to polar coordinates, $[r, \theta]$, of a standard bivariate normal $[x, y] \sim (1/2\pi)\exp((-1/2)(x^2 + y^2))$.

$$[r, \theta] \sim \frac{1}{2\pi}\exp\left(\frac{-r^2}{2}\right)\left|\begin{array}{cc} \cos(\theta) & \sin(\theta) \\ -r\sin(\theta) & r\cos(\theta) \end{array}\right| = \frac{1}{2\pi}\,r\exp\left(\frac{-r^2}{2}\right) \ .$$

Hence, r and θ are independent, θ is uniformly distributed in $[0, 2\pi]$, and r^2 is a χ_2^2 variate. Finally, we see that r is produced by the transformation defined in item (d) above to generate a χ_2^2 variate.

If the scaled density, κg, can be used as an *envelope* dominating the density f, that is, $f \leq \kappa g$, the following *acceptance-rejection* method due to von Neumann can be used: (1) Generate $[y_i, u_i] \sim g \times U_{[0,1]}$ until $\kappa u_i \leq f(y_i)/g(y_i)$. (2) Take $x_i = y_i$.

The Gamma distribution with parameter c is $f(x) = x^{c-1}\exp(-x)/\Gamma(c)$. For $c = 1$ this is the exponential distribution, also, the sum of two gamma variates with parameters c_1, c_2 is a gamma variate with parameter $c_1 + c_2$. The following results given in Deák (1990, sec.4.5) provide implicit acceptance rejection generation methods:

(i) For $c < 1$, $f(x)$ is dominated by the following density $g(x)$ scaled by the factor $\kappa = (c\Gamma(c))^{-1} + (e\Gamma(c))^{-1}$. Moreover, G^{-1} has an easy analytic form.

$$g(x) = \left\{\begin{array}{l} \frac{ec}{(e+c)}x^{c-1}, \text{ if } x \in [0, 1] \\ \frac{ec}{(e+c)}e^{-x}, \text{ if } x \in [1, \infty[\end{array}\right. , \quad G(x) = \left\{\begin{array}{l} \frac{e}{(e+c)}x^c, \text{ if } x \in [0, 1] \\ \frac{e}{(e+c)} + \frac{c}{(e+c)}(1 - e^{1-x}), \text{ if } x \in [1, \infty[\end{array}\right.$$

(ii) For $c > 1$, $f(x)$ is dominated by a Cauchy with parameters $a = 1/\sqrt{2c-1}$ and $b = c - 1$, scaled by the factor $\kappa = \pi\sqrt{2c-1}\exp(-c+1)(c-1)^{c-1}/\Gamma(c)$.

(iii) For $c > 1$, $f(x)$ is dominated by the envelope density, $g_c(x)$, and scale factor, κ_c, described as follows. First, let us consider an auxiliar variate distributed as the t-density with 2 degrees of freedom. The auxiliar density, $g(y)$, cumulative distribution, $G(y)$, and generation method by direct inversion are as follows:

$$g(y) = \frac{1}{2\sqrt{2}}\left(1 + \frac{y^2}{2}\right)^{-\frac{3}{2}} \ , \quad G(y) = \frac{1}{2}\left(1 + \frac{y/\sqrt{2}}{\sqrt{1 + y^2/2}}\right) \ , \quad y \sim \frac{\sqrt{2}(u - 1/2)}{\sqrt{u(1 - u)}} \ .$$

Next, let us consider the envelope variate with density and scale factor defined as

$$\frac{1}{\kappa_c \, g_c(x)} = \Gamma(c) \left(1 + \frac{1}{2} \left(\frac{x - (c-1)}{\sqrt{3c/2 - 3/8}} \right)^2 \right)^{3/2} ,$$

$$\kappa_c = \frac{2}{\Gamma(c)} \sqrt{3c - \frac{3}{4}} \left(\frac{c-1}{e} \right)^{c-1} \leq \sqrt{\frac{6}{\pi}} \, e^{1/c} .$$

The envelope variate can be generated from the auxiliar variate as

$$x \sim (c-1) + y\sqrt{3c - 3/4} .$$

(iv) It is easy to check that if y is a gamma variate with parameter $c+1$ and u is uniform in $[0, 1[$, than $x = yu^{1/c}$ is a gamma variate with parameter c. This property can be used to use a gamma generator in the domain $c < 1$ to generate a gamma variate with parameter $c > 1$, and vice-versa.

Appendix B presents characterizations of the Beta an Dirichlet distributions by the Gamma, hence providing implicit generation mechanisms for those distributions. For more non-uniform random generation methods see Deák (1990), Gentle (1998), Lange (2000), Ripley (1987), and the encyclopedic work of Fishman (1996).

G.3   MCMC - Markov Chain Monte Carlo

This section uses the matrix notation and the basic facts about homogeneous Markov chains reviewd in section H.1.

Markov Chain Monte Carlo, Conditional Monte Carlo, etc. are common names for methods that generate indirect random sampling for a discrete target density g. MCMC sampling is based on a Markov chain that has the target density as its limit distribution. Our presentation follows ch.1 of Gilks et al. (1996). For the original papers, see Geman and Geman (1984), Hastings (1970), Metropolis and Ulam (1949), and Metropolis et al. (1953).

The basic idea of the MCMC algorithms is to adapt a general (irreducible and aperiodic) sampling kernel, Q, to the desired target distribution, $g > 0$. Starting form state i, the MCMC algorithm proceeds as follows:
(1) A candidate for the next state, j, is proposed with probability Q_i^j.
(2a) The chain moves to the candidate j with *acceptance probability* $\alpha(i, j)$.
(2b) Otherwise, candidate j is rejected, and the chain remains at state i.
(3) Go to step 1.
Formally, the MCMC transition kernel, P, has the form

$$P_i^j = Q_i^j \alpha(i, j) + I(j = i) \left(1 - \sum_j Q_i^j \alpha(i, j) \right) ,$$

where the first term corresponds to the acceptance of new state j, while the second term corresponds to the rejection of the proposed candidate, indicating that the chain remains at state i.

In order to obtain the target distribution, g, as the limit distribution of the MCMC, we want to choose an acceptance probability, $\alpha(i,j)$, that enforces the detailed balance equation,

$$g^i P_i^j = g^i Q_i^j \alpha(i,j) = g^j Q_j^i \alpha(j,i) = g^j P_j^i \ .$$

It is easy to check that the acceptance probabilities suggested by Metropolis-Hastings and Barker accomplish the goal. They are, respectively,

$$\alpha(i,j) = \min\left(1\,,\ \frac{g^j Q_j^i}{g^i Q_i^j}\right) \quad \text{and} \quad \alpha(i,j) = \frac{g^j Q_j^i}{g^i Q_i^j + g^j Q_j^i}\ ,$$

In Bayesian statistics, MCMC methods are typically used to compute $\widehat{f}$, the expected value of a function, $f(\theta)$, on a specific region of the parameter space, $T \subseteq \Theta$, with respect to the posterior density, $p_n(\theta)$. In standard Bayesian models, $p_n(\theta) = c(y)^{-1} L(\theta \,|\, y) p_0(\theta)$, where $p_0(\theta)$ is the prior distribution of the parameter θ, $L(\theta \,|\, y)$ is the likelihood of θ given the observed data y, and $c(y)$ is the posterior normalization constant. Hence,

$$\widehat{f} = \frac{1}{c(y)} \int_T f(\theta) g(\theta \,|\, y) d\theta \ , \ \ g(\theta) = L(\theta \,|\, y) p_0(\theta) \ , \ \ c(y) = \int_\Theta g(\theta \,|\, y) d\theta \ .$$

Notice that $\alpha(i,j)$, the acceptance probabilities defined above, can be computed from posterior ratios $p_n(\theta^j)/p_n(\theta^i) = g^j/g^i$. Hence, actual implementations of these MCMC algorithms do not require the explicit knowledge of the target distribution normalization constant, $c(y)$. It suffices to have an un-normalized function that is proportional to the target distribution, $g(\theta) \propto p_n(\theta)$, as it is the case for the likelihood-prior product.

The original Metropolis algorithm uses a symmetric sampling kernel, $Q_i^j = Q_j^i$, see Metropolis et al. (1954). In this caese, Metropolis-Hastings acceptance probability can be simplified to the form $\alpha(i,j) = \min(1, g^j/g^i)$. In statistical physics, the density of interest, g^i, often takes the form of the Boltzmann distribution, $g^i = \exp(-\beta H(i))$, where the Hamiltonian function, $H(i)$, gives the energy of the corresponding state. In this case, a new state of lower energy, $j \,|\, \Delta H = H(j) - H(i) \leq 0$, is accepted for sure, while a state of higher energy is accepted with probability $\exp(-\beta \Delta H)$. In section H.1, the same acceptance rejection mechanism reappears in Metropolis version of Simulated Annealing.

Random Walk Metropolis algorithms use a symmetric kernel that is a function only of the random walk step, $z = y - x$, that is, $Q(x,y) = Q(z) = Q(-z)$. A common option in practical implementations is to chose the random walk step from a multivariate Normal distribution, $z \sim N(0, \Sigma)$. The covariance matrix, Σ, scales the random walk steps. If the steps are too large, the proposed steps would often result in sharp decrease of the traget density, so the acceptance rate is low, making the MCMC inefficient. If the steps

are too small, the acceptance rate may be high, but too many steps are required to move effectively across the integration region and, again, the MCMC is inefficient.

A practical solution is to take the covariance matrix, Σ, proportional to the inverse Hessian matrix, $(-\partial^2 \log g(x)/\partial x' \partial x)^{-1}$, computed at the estimated mode, $\widehat{x} = \arg\max g(x)$. Alternatively, one can take Σ proportional to a convex combination of the diagonal matrix D, a prior estimate of marginal variances, and the current estimate of the sampled covariance matrix.

$$\Sigma \propto (1-\lambda)S + \lambda D \;,\;\; S = \frac{1}{n}\sum_{j=1}^{n}(x^j - \bar{x})(x^j - \bar{x})' = \frac{1}{n}(X - \bar{x})(X - \bar{x})' \;.$$

In both cases, the proportionality constant is interactively adapted in order to obtain an acceptance rate in a specified range. If the target distribution has heavy tails, this sampling kernel may be modified to a multivariate student's t-distribution. For furthe details, see Gilks et al. (1996).

Cyclic MCMC schemes use a "composit kernel" that updates, one by one, the individual components of a k-dimensional vector state, x. That is, a cyclic MCMC goes from the current state, x to the next state, y, by k intermediate steps, $x = [x_1, x_2, \ldots x_k]$, $[y_1, x_2, \ldots x_k]$, $[y_1, y_2, \ldots x_k]$, $\ldots [y_1, y_2, \ldots y_k] = y$. Cyclic schemes include the Gibbs sampler, popularized by Geman and Geman (1984), and many useful variations.

G.4 Estimation of Ratios

This section presents the derivation of the Monte Carlo procedure for the numerical integrations required to implement the FBST. The symbol X represents the observed data or some sufficient statistics. The best approach to the numerical integration step required by the FBST is approximation by Monte Carlo (MC) simulation, see Appendix A for the FBST definition, and Evans and Swartz (2000) and Zacks and Stern (2003) for the Monte Carlo approach to this integration problem. We want an estimate of the ratio

$$\mathrm{ev}(H; X) \;\; = \;\; \frac{\int_{\overline{T}} f(\theta; X)d\theta}{\int_{\Theta} f(\theta; X)d\theta}$$

$$\overline{T} = \overline{T}(s^*) \;,\;\; \overline{T}(v) = \{\theta \in \Theta \,|\, s(\theta) > v\} \;.$$

Since the space Θ is unbounded, we randomly chose the values of θ according to an "importance sampling" density $g(\theta)$, which is positive on Θ. The evidence function is equivalent to

$$\mathrm{ev}(H; X) \;\; = \;\; \frac{\int_{\Theta} Z_g^*(\theta; X)g(\theta)d\theta}{\int_{\Theta} Z_g(\theta; X)g(\theta)d\theta}$$

where

$$
\begin{aligned}
Z_g(\theta; X) &= \frac{f(\theta; X)}{g(\theta)} \quad \text{and} \\
Z_g^*(\theta; X) &= I^*(\theta; X) Z_g(\theta; X) \\
I^*(\theta; X) &= 1(\theta \in \overline{T})
\end{aligned}
$$

Thus, a Monte Carlo estimate of the evidence is

$$
\hat{E}v_{g,m}(X) = \frac{\sum_{j=1}^m Z_g^*(\theta^j; X)}{\sum_{j=1}^m Z_g(\theta^j; X)}
$$

where $\theta^j, j = 1 \ldots m$ are iid and independently chosen in Θ according to the importance sampling density $g(\theta)$. Thus,

$$
\hat{E}v_{g,m}(X) \overset{m \to \infty}{\Longrightarrow} \text{ev}(H; X) \quad \text{a.s.}[g]
$$

The goodness of the MC estimation depends on the choice of g and m. Standard statistical software libraries have univariate random generators for most common distributions. These univariate generators can also be used to build vector variates from multivariate distributions. Appendix D describes how to generate a Dirichlet vector variate from univariate Gammas.

Johnson (1980) describes a simple procedure to generate the Cholesky factor of a Wishart variate $W = U'U$ with n degrees of freedom, from the Cholesky factorization of the covariance parameter $V = R^{-1} = C'C$:

$$
\begin{aligned}
L_i^j &= N(0, 1) \;, \; i > j \\
L_i^i &= \sqrt{\chi^2(n - i + 1)} \;; \; U = L'C
\end{aligned}
$$

At the integration step it is important to perform all matrix computations directly from Cholesky factors, Golub and van Loan (1989), Jones (1985). In this problem we can therefore use "exact sampling", what simplifies substantially the integration step, i.e., $Z_g(\theta; X) = 1$.

Precision of the MC Simulation

In order to control the number of points, m, used at each MC simulation, we need an estimate of MC precision for evidence estimation. For a fixed large value m, the asymptotic distribution of $\hat{E}v_{g,m}(X)$ is normal with mean $\text{ev}(H; X)$ and asymptotic variance $V_g(X)$. According to the delta method, Bickel and Doksum (2001), we obtain that

$$
V_g(X) = \frac{1}{m} \left(\frac{\sigma_g^{*2}}{\mu_g^2} + \frac{\sigma_g^2 \mu_g^{*2}}{\mu_g^4} - 2 \frac{\mu_g^*}{\mu_g^3} \gamma_g \right)
$$

where

$$\mu_g = \int_\Theta Z_g(\theta; X) g(\theta) d(\theta)$$

$$\mu_g^* = \int_\Theta Z_g^*(\theta; X) g(\theta) d(\theta)$$

$$\sigma_g{}^2 = \int_\Theta \left(Z_g(\theta; X) - \mu_g\right)^2 g(\theta) d(\theta)$$

$$\sigma_g^{*2} = \int_\Theta \left(Z_g^*(\theta; X) - \mu_g^*\right)^2 g(\theta) d(\theta)$$

$$\gamma_g{}^2 = \int_\Theta \left(Z_g(\theta; X) - \mu_g\right) \left(Z_g^*(\theta; X) - \mu_g^*\right) g(\theta) d(\theta)$$

are the expected values, variances and covariance of $Z(\theta; X)$ and $Z^*(\theta; X)$ with respect to $g(\theta)$.

Define the coefficients

$$\xi_g = \frac{\sigma_g}{\mu_g} , \quad \xi_g^* = \frac{\sigma_g^*}{\mu_g}$$

For abbreviation, let $\eta = \mathrm{ev}(H; X)$. Also note that $\eta = \mu_g^*/\mu_g$. Then the asymptotic variance is

$$V_g(X) = \frac{1}{m}\left(\xi_g^{*2} + \eta^2\xi_g{}^2 - 2\frac{\eta\,\gamma_g}{\mu_g{}^2}\right)$$

Let us define the complementary variables

$$Z_g^c(\theta; X) = I^c(\theta; X) Z_g(\theta; X)$$
$$I^c(\theta; X) = 1 - I^*(\theta; X)$$
$$\sigma_g^{c2} = V_g\left(Z^c(\theta; X)\right)$$
$$\xi_g^c = \frac{\sigma_g^c}{\mu_g}$$

Some algebraic manipulation give us $V_g(X)$ in terms of ξ_g^* and ξ_g^c, namely

$$V_g(X) = \frac{1}{m}\left(\xi_g^{*2}(1-\eta)^2 + \xi_g^{c2}\eta^2 + 2\,\eta^2(1-\eta)^2\right)$$

For large values of m, the asymptotic $(1 - \beta)$ level confidence level confidence interval for η is $\hat{E}v_{g,m}(X) \pm \Delta_{g,m,\beta}$, where

$$\Delta_{g,m,\beta}^2 = \frac{F_{1-\beta}(1, m)}{m}\left(\hat{\xi}_g^{*2}(1-\hat{\eta})^2 + \hat{\xi}_g^{c\,2}\hat{\eta}^2 + 2\hat{\eta}^2(1-\hat{\eta})^2\right)$$

where $F_{1-\beta}(1, m)$ is the $1 - \beta$ quantile of the $F(1, m)$ distribution, and $\hat{\eta}$, $\hat{\xi}_g^*$ and $\hat{\xi}_g^c$ are consistent estimators of the respective quantities.

For large m, we can also use the approximation,

$$\Delta_{g,m,\beta}^2 \;\; = \;\; \frac{\chi_{1-\beta}^2(1)}{m} \left(\hat{\xi}_g^{*2}(1 - \hat{\eta})^2 + \hat{\xi}_g^{c\,2}\hat{\eta}^2 + 2\,\hat{\eta}^2(1 - \hat{\eta})^2 \right)$$

since $F(1, m)$ converges in distribution to the chi-square distribution with 1 degree of freedom, as $m \to \infty$.

If we wish to have $\Delta_{g,m,\beta} \leq \delta$, for a prescribed value of δ, then m should be such that

$$m \;\; \geq \;\; \frac{\chi_{1-\beta}^2(m)}{\delta^2} \left(\hat{\xi}_g^{*2}(1 - \hat{\eta})^2 + \hat{\xi}_g^{c\,2}\hat{\eta}^2 + 2\,\hat{\eta}^2(1 - \hat{\eta})^2 \right)$$

G.5   Monte Carlo for Linear Systems

Want to solve the simultaneous matrix equation,

$$x = Hx + b , \quad H \; n \times n$$

The (Direct) Monte Carlo methods of von Neumann and Ulam (NU) and of Wasow (WS) are based on probability transitions, P_i^j, and multipliers or weights, V_i^j, satisfying the following conditions:

$$V_i^j = (H_i^j / P_i^j) I(P_i^j > 0) \; | \; \; H_i^j \neq 0 \Rightarrow P_i^j > 0 \; \wedge \; P_{1:n}^{1:n} \mathbf{1} < \mathbf{1}$$

We also define the extended Stochastic matrix,

$$P = \begin{bmatrix} P_1^1 & \cdots & P_1^n & P_1^{n+1} \\ \vdots & & \vdots & \vdots \\ P_n^1 & \cdots & P_n^n & P_n^{n+1} \\ 0 & \cdots & 0 & 1 \end{bmatrix} , \quad P_i^{n+1} = 1 - \sum_{j=1}^n P_i^j$$

P defines a Markov chain in a space of $n+1$ states, $\{1, 2, \ldots n, n+1\}$, where the last state, $n+1$, is an absorbing state.

We want to consider a random path or trajectory, T, of a "particle" starting at state i, until the particle is absorbed at step $m+1$, that is,

$$T = [T(1) = i, T(2), \ldots, T(m), T(m+1) = n+1]$$

We define a random variable, $X(T)$, associated to each trajectory.

First we define the multipliers products

$$v_1 = 1 \; \; \text{and} \; \; v_k = v_{k-1} V_{T(k-1)}^{T(k)} , \; \; 2 \leq k \leq m .$$

Von Neumann - Ulam's and Wasow's versions of the Monte Carlo Algorithm, use $X(T)$ equal to, respectively,

$$NU(T) = v_m b_{T(m)} / P_{T(m)}^{n+1} \; \; \text{and} \; \; WS(T) = \sum_{k=1}^m v_k b_{T(k)} .$$

The key to these Monte Carlo algorithm is that the expected value of the variable $X(T)$, over all trajectories starting at state i, is the solution of the simultaneous equation, provided these expected values are well defined, that is, if

$$\text{if} \; \; e_i = E(X(T) \, | \, T(1) = i) \; \; \text{then} \; \; e = He + b$$

Let us prove the statement above for Wasow's version. By definition,

$$\Pr(T) = \prod_{k=1}^{m} P_{T(k)}^{T(k+1)} \quad \text{and}$$

$$e_i = \sum_{\substack{T = [T(1) = i, T(2) = j, \dots T(m+1) = n+1] , \\ m = 1, 2, \dots \infty .}} X(T)\Pr(T) .$$

Given a trajectory T, we can separate the terms in $X(T)$ with index 1, that is,

$$X(T) = b_{T(1)} + V_{T(1)}^{T(2)} X(T(2:m+1)) , \quad \text{hence,}$$

$$e_i = \sum_{j=1}^{n+1} P_i^j \sum_{S=[j,\dots n+1]} \left(b_i + V_i^j X(S)\right) \Pr(S)$$

$$= \sum_{j=1}^{n} P_i^j \sum_{S=[j,\dots n+1]} \left(b_i + V_i^j X(S)\right) \Pr(S) + P_i^{n+1} b_i$$

$$= \sum_{j=1}^{n} P_i^j V_i^j \sum_{S=[j,\dots n+1]} X(S)\Pr(S) + b_i \left(P_i^{n+1} + \sum_{j=1}^{n} P_i^j \sum_{S} \Pr(S) \right)$$

$$= \sum_{j=1}^{n} H_i^j e_j + b_i , \quad \text{Q.E.D.}$$

The Reverse or Adjoint Monte Carlo methods of von Neumann and Ulam (NU) and of Wasow (WS) are based on probability transitions, Q_i^j, and multipliers or weights, W_i^j, satisfying the following conditions:

$$W_i^j = (H_j^i/Q_i^j)I(Q_i^j > 0) \mid H_j^i \neq 0 \Rightarrow Q_i^j > 0 \ \wedge \ Q_{1:n}^{1:n}\mathbf{1} < \mathbf{1}$$

We also define the extended Stochastic matrix,

$$Q = \begin{bmatrix} Q_1^1 & \cdots & Q_1^n & Q_1^{n+1} \\ \vdots & & \vdots & \vdots \\ Q_n^1 & \cdots & Q_n^n & Q_n^{n+1} \\ 0 & \cdots & 0 & 1 \end{bmatrix} , \quad Q_i^{n+1} = 1 - \sum_{j=1}^{n} Q_i^j$$

We want to consider a random path or trajectory, T, of a "particle" starting at state i, chosen at random with probability r_i, until the particle is absorbed at step $m+1$, just after visiting state $T(m)$ at step m , that is,

$$T = [T(1) = i, T(2), \dots, T(m), T(m+1) = n+1]$$

We define random variables associated to each trajectory. First we define the multiplier products

$$w_1 = b_i/r_i \quad \text{and} \quad w_k = w_{k-1} W_{T(k-1)}^{T(k)} \ , \ 2 \leq k \leq m \ .$$

Von Neumann - Ulam's and Wasow's versions of the reverse or adjoint Monte Carlo Algorithm, use $X_j(T)$ equal to, respectively,

$$NU_j(T) = w_m \delta_{T(m)}^j / Q_{T(m)}^{n+1} \quad \text{and} \quad WS_j(T) = \sum_{k=1}^{m} w_k \delta_{T(k)}^j \ .$$

Again, the key to these Monte Carlo algorithm is that the expected value of the variable $X_j(T)$, over all trajectories ending at state j, is the solution of the simultaneous equation, provided these expected values are well defined. The proof for the reverse method is similar to the direct case.

Appendix H

Stochastic Evolution and Optimization

> *"God does not play dice (with the universe)."*
>
> Albert Einstein (1879 - 1955).

> *"Einstein, stop telling God what to do (with his dice)."*
>
> Niels Bohr (1885 - 1962).

> *"God not only plays dice, He also sometimes throws the dice where they are not seen."*
>
> Stephen Hawking (1942 -   ).

This section gives a condensed introduction to inhomogeneous Markov chains, the theory that is needed to formalize Simulated Annealing (SA) and related algorithms presented in chapter 5. We follow the presentations in Jetschke (1989) and Pflug (1996, ch.2), and assume some familiarity with homogeneous Markov chains, as presented in Feller (1957, ch.15) or Häggström (2002).

H.1   Inhomogeneous Markov Chains

We begin by introducing some notation for this chapter. First, a notational idiosyncrasy: In almost all areas of mathematics it is usual to write a d-dimensional vector as a $d \times 1$ *column matrix*, x, and a linear transformation as the left multiplication of x by a $d \times d$

square matrix A, that is, Ax. However, in the literature of Markov chains, it is usual to write a a d-dimensional vector as a $1 \times d$ or *row matrix*, v, and a linear transformation as the right multiplication of v by a $d \times d$ square matrix P, that is, vP. Herein, we make use of the two forms, according to the context.

d-Dimensional vectors are written in lower case format, v. A density or probability vector is a vector in the simplex support, $v > 0$ and $\|v\| = 1$. d-Dimensional (square) matrices, on the other hand, are written in upper case format, P. In particular, I will reserved to denote the d-dimensional identity matrix. A d-dimensional kernel or transition probability matrix has its rows in the simplex support. Right subscripts and superscripts will index matrices rows and columns. For instance, P_i, P^j and P_i^j will indicate the i-th row, the j-th column, and the element or entry i, j of matrix P, respectively. In the same way, x_i and v^j denote, respectively, the i-th element of the column vector x, and the j-th element of the row vector v.

Braces are used to index a sequence of objects, such as $P\{1\}, P\{2\}, \ldots P\{t\}$. The symbol $P\{s::t\}$ will denote the product of the objects indexed from s to t, that is,

$$P\{s::t\} \equiv \prod_{k=s}^{t} P\{k\} \ .$$

Finaly, given scalars, α and β, we have, as usual, $\alpha \wedge \beta = \min(\alpha, \beta)$, $\alpha \vee \beta = \max(\alpha, \beta)$, $\alpha^+ = 0 \vee \alpha$, $\alpha^- = 0 \vee -\alpha$.

Homogeneous Markov Chains

In a Markov chain with kernel or transition matrix P, $P_i^j \geq 0$ such that $P_i \mathbf{1} = 1$, P_i^j represents transition probability from state $x\{i\}$ to state $x\{j\}$ in a finite state space, $S = \{x\{1\}, x\{2\}, \ldots x\{d\}\}$. For the sake of simplicity, we often write the index, i, instead of the indexed state, $x\{i\}$, that is, we identify the state space with its index set, $S = \{1, 2, \ldots d\}$.

A trajectory or path of length t from an initial state i to a final state j is given by $\tau = [\tau(1) = i, k(2), \ldots \tau(t), \tau(t+1) = j]$. If a Markov chain is initially at state i, the probability that it will follow the trajectory τ is

$$\Pr(\tau) = \prod_{k=1}^{t} P_{\tau(k)}^{\tau(k+1)}$$

If we select the initial state state, i, from distribution v, $v \geq 0$, $v\mathbf{1} = 1$, the probability that the chain is at state j after t transitions, following any possible trajectories trough intermediate states, is given by w^j, where

$$w = v \prod_{k=1}^{t} P \ .$$

A trajectory τ is possible if it has non-zero probability. A Markov chain is irreducible if there is a possible trajectory connecting any initial state, i, to any final state, j. A cycle is a trajectory with the same initial and final states. State i has period $k > 1$ if any possible cycle starting at i has length multiple of k. Otherwise, state i is aperiodic. A Markov chain is aperiodic if has no periodic states.

The probability distribution g is invariant by kernel P if $g = gP$. An invariant distribution is also known as eigen-solution, equilibrium or stable distribution for P. It can be shown that an irreducible and aperiodic Markov chain has a unique invariant distribution, see Feller (1957). Under the same regularity conditions, it can also be shown that the invariant distribution is the chain's limiting distribution, that is,

$$
\lim_{t \to \infty} \prod_{k=1}^{t} P \;=\;
\begin{bmatrix} g \\ g \\ \vdots \\ g \end{bmatrix}
\;=\;
\begin{bmatrix}
g^1 & g^2 & \cdots & g^d \\
g^1 & g^2 & \cdots & g^d \\
\vdots & \vdots & & \vdots \\
g^1 & g^2 & \cdots & g^d
\end{bmatrix} .
$$

Hence, for any initial distribution, v,

$$
v \left(\lim_{t \to \infty} \prod_{k=1}^{t} P \right) \;=\; g \ .
$$

Given the irreducible and aperiodic kernel P, having the stable distribution g, the *reverse* kernel, R, is defined as $R_i^j = g^j P_j^i / g^i$. The reverse kernel can be interpreted, using Bayes theorem, as the kernel of the Markov chain P going backwards in time, that is,

$$
R_i^j = \Pr(x\{t\} = j \,|\, x\{t+1\} = i) = \frac{\Pr(x\{t+1\} = i \,|\, x\{t\} = j)\Pr(x\{t\} = j)}{\Pr(x\{t+1\} = i)} = \frac{P_j^i g^j}{g^i} \ .
$$

Kernel P is *reversible* if there is a distribution g statisfying the *detailed balance equation*, $g^i P_i^j = g^j P_j^i$. Summing both sides of the detailed balance equation over index i, we obtain $g^j = \sum_i g^i P_i^j$, showing that this is a sufficient condition for g to be an invariant distribution. Hence, for a reversible chain, the forward and backward kernels are identical, $R_i^j = P_i^j$.

Vector and Matrix Norms

A **norm**, in a vector space E, is a function

$$
\| \, . \, \| \; : \; E \Rightarrow \mathbf{R} \,|\, \forall x, y \in E \ \text{and} \ \alpha \in \mathbf{R} \ ,
$$

1. $\|x\| \geq 0, \ \text{and} \ \|x\| = 0 \Leftrightarrow x = 0.$

2. $\|\alpha x\| = |\alpha| \, \|x\|.$

3. $\|x + y\| \leq \|x\| + \|y\|$, the triangular inequality.

In particular, for $x \in \mathbf{R}^n$ and $p > 0$,

$$\|x\|_p = \left(\sum_1^n |x_i|^p\right)^{1/p} \quad , \quad \|x\|_\infty = \max_{i=1}^n |x_i| \ .$$

defines the standard L_p norms in $\mathbf{R}^n$.

Given a normed vector space, $(E, \|\ \|)$,

$$\|T\| \equiv \max_{x \neq 0}(\ \|T(x)\| \ / \ \|x\| \ ) \ .$$

defines the **induced norm** on the vector space of linear transformations, $T : E \to E$, for which $\exists \alpha \in \mathbf{R} \ | \ \|T(x)\| \leq \alpha\|x\|, \ \forall x \in E$, that is, the vector space of bounded linear transformations on E. By linearity,

$$\|T\| \equiv \max_{x|\ \|x\|=1} \|T(x)\| \ .$$

In $(\mathbf{R}^n, \|\ \|)$ the induced norm on set of bounded linear transformations, $T : \mathbf{R}^n \to \mathbf{R}^n$, defines the matrix norm in $(\mathbf{R}^n, \|\ \|)$. Speciffically, for an $n \times n$ matrix A, $\|A\| = \|T\|$, where $T(x) = Ax$.

Lemma 1: The matrix norm in $(\mathbf{R}^n, \|\ \|)$, has the following properties: If A and B are $n \times n$ matrices,

1. $\|A\| \geq 0$ and $\|A\| = 0 \Leftrightarrow A = 0$

2. $\|A + B\| \leq \|A\| + \|B\|$

3. $\|AB\| \leq \|A\| \ \|B\|$

Lemma 2: (L_1 and L_∞ explicit expressions).

$$\|A\|_1 \ = \ \max_{j=1}^n \sum_{i=1}^n |A_i^j|$$

$$\|A\|_\infty \ = \ \max_{i=1}^n \sum_{j=1}^n |A_i^j|$$

Proof: To check the expression for L_1 and L_∞ observe that

$$\|Ax\|_1 \ = \ \sum_{i=1}^n |\sum_{j=1}^n A_i^j x_j| \ \leq \ \sum_{i=1}^n \sum_{j=1}^n |A_i^j| \ |x_j|$$

$$\leq \ \sum_{j=1}^n |x_j| \max_{j=1}^n \sum_{i=1}^n |A_i^j| \ = \ \|A\|_1 \ \|x\|_1$$

$$\|Ax\|_\infty \ = \ \max_{i=1}^n |\sum_{j=1}^n A_i^j x_j| \ \leq \ \max_{i=1}^n \sum_{j=1}^n |A_i^j| \ |x_j|$$

$$\leq \ \max_{j=1}^n |x_j| \max_{i=1}^n \sum_{j=1}^n |A_i^j| \ = \ \|x\|_\infty \ \|A\|_\infty$$

and that, if k is the index that realizes the maximum in the norm definition, then the equality is realized by the vector $x = I^k$ for L_1, and by the vector $x \mid x_j = sig(A_i^j)$ for L_∞.

One can check that $\|x\|_\infty \le \|x\|_1 \le n\|x\|_\infty$ and $\|x\|_\infty \le \|x\|_2 \le n^{1/2}\|x\|_\infty$. In fact, any given p norn can provide a bound to another q norm and, in this sense, they are equivalent. In the remaining of this section the L_1 norm will be used throughout, so we will write $\|x\|$ for $\|x\|_1$.

Dobroushin's Contraction Coefficient

Lemma 3 (Total Variation). Given two probability (non-negative, unitary, row) vectors, v and w, their Total Variation or L_1 difference has the alternative expressions:

$$\|v - w\| = 2\left(1 - \sum_k v^k \wedge w^k\right) = 2\sum_k \left(v^k - w^k\right)^+$$

Proof: Just notice that

$$2 - 2\sum_k v^k \wedge w^k = \sum_k v^k + \sum_k w^k - 2\sum_k v^k \wedge w^k = \sum_k |v^k - w^k| \,, \quad \text{and}$$

$$\left(v^k - w^k\right)^+ = \left(v^k - v^k \wedge w^k\right) \text{ hence } \sum_k \left(v^k - w^k\right)^+ = 1 - \sum_k v^k \wedge w^k \,.$$

The Dobroushin Contraction Coefficient or Ergodicity Coefficient of a transition probability matrix, P, is defined as

$$\rho(P) \equiv \frac{1}{2}\max_{i,j}\sum_k |P_i^k - P_j^k| = \frac{1}{2}\max_{i,j}\|I_iP - I_jP\| \,.$$

It is clear from the definition that $\rho(P)$ measures the maximum L_1 distance between the rows of P. If a sequence of kernels, $P\{k\}$, is clear from the context, we shall also write

$$\rho\{k\} \equiv \rho(P\{k\}) \,, \quad \text{and} \quad \rho\{m::n\} \equiv \prod_{k=s}^t \rho\{k\} \,.$$

Lemma 4 (Vector Contraction). Two probability vectors, v and w, are contracted by the transition matrix P in the sense that:

$$\|vP - wP\| \le \rho(P)\|v - w\| \,.$$

Proof: If $v = w$ or if $v = I_i$ and $w = I_j$, the result is trivial. Otherwise, let $v \ne w$ and $m = v \wedge w$. Defining

$$G_i^j = 2\frac{(v_i - m_i)(w_j - m_j)}{\|v - w\|} \,,$$

it is easy to check that:

(a) $G_i^j \geq 0$,

(b) $v - w = \sum_{i,j} G_i^j (I_i - I_j)$, and

(c) $\frac{1}{2} \|v - w\| = \sum_{i,j} G_i^j$.

Hence,

$$\|vP - wP\| = \|\sum_{i,j} G_i^j (I_i - I_j)P\| \leq$$

$$\left(\sum_{i,j} G_i^j\right) \max_{i,j} \|(I_i - I_j)\| = \frac{1}{2}\|v - w\|2\rho(P) = \rho(P)\|v - w\| .$$

Lemma 5 (Matrix Contraction). Two transition matrices, P and Q, are contracted in the sense that:

$$\rho(PQ) \leq \rho(P)\,\rho(Q) .$$

Proof:

$$\rho(PQ) \;=\; \frac{1}{2} \max_{i,j} \|(I_i - I_j)PQ\| \leq \rho(Q)\frac{1}{2} \max_{i,j} \|(I_i - I_j)P\| = \rho(P)\,\rho(Q) .$$

Theorem 6 (Weak Ergodicity (loss of memory)).

$$\lim_{t\to\infty} \rho\{1::t\} = 0 \Rightarrow \lim_{t\to\infty} \|(v - w)\,P\{1::t\}\| = 0 .$$

Proof: Immediate, from Lemma 2.

Lemma 7 (Strong Ergodicity). Assume that the following conditions hold:

(a) Each $P\{k\}$ has a unique invariant distribution, $v\{k\} = v\{k\}\,P\{k\}$, such that $\sum_{k=1}^{\infty} \| v\{k+1\} - v\{k\}\| < \infty$;

(b) $\rho\{k\} > 0$;

(c) $\rho\{1::\infty\} = 0$.

Then, there is a limiting distribution, $v\{\infty\}$, such that, for any distribution w,

$$\lim_{t\to\infty} \| wP\{1::t\} - v\{\infty\}\| = 0$$

Proof. Condition 7a ensures that, with respect to the L_1 norm, $v\{k\}$ is a Cauchy sequence in the compact simplex support. Hence, the sequence has a unique accumulation point, $v\{\infty\} = \lim_{k\to\infty} v\{k\}$.

Since for $1 < s < t < \infty$

$$v\{\infty\}\,P\{s::t\} - v\{\infty\} = (v\{\infty\} - v\{s\})\,P\{s::t\} + v\{s\}\,P\{s::t\} - v\{\infty\} =$$

$$(v\{\infty\} - v\{s\})\,P\{s::t\} + \sum_{k=s}^{t-1} (v\{k\} - v\{k+1\})\,P\{k+1::t\} + v\{t\} - v\{\infty\} ,$$

we have the inequality

$$\|wP\{1::t\} - v\{\infty\}\| \le \|(wP\{1::t-1\} - v\{\infty\})P\{s::t\}\| + \|v\{\infty\}P\{s::t\} - v\{\infty\}\| \le$$

$$2\rho\{s::t\} + \|v\{\infty\} - v\{s\}\| + \sum_{k=s}^{n-1}\|v\{k\} - v\{k+1\}\| + \|v\{\infty\} - v\{t\}\| \le$$

$$2\rho\{s::t\} + 2\sup_{k \ge s}\|v\{\infty\} - v\{k\}\| + \sum_{k=s}^{t-1}\|v\{k\} - v\{k+1\}\| \ .$$

Letting $t \to \infty$, all terms in the right hand side can be made arbitrarily small for an appropriate large value of s. Consequently, the left hand side converges to zero, Q.E.D.

Theorem 8 (Small Perturbations). It is possible to use a perturbed sequence of kernels, $Q\{k\}$, instead of $P\{k\}$, and still obtain convergence to the same invariant distribution provided that

$$\sum_{k=1}^{\infty}\|P\{k\} - Q\{k\}\| < \infty \ .$$

Proof. The result follows from the inequality

$$\|P\{s::t\} - Q\{s::t\}\| \le \sum_{k=s}^{t}\|P\{k\} - Q\{k\}\|$$

The Small Perturbations theorem plays an important role in the design of efficient algorithms based on heuristic perturbations, a technique that can greatly expedite the annealing process, see Stern (1991) and Pflug (1996, ch.2).

H.2 Simulated Annealing

The Metropolis Algorithm

Consider a system, X, where the system state is parameterized by a d-dimentional coordinate vector $x = [x_1, \ldots x_d] \in X$. The neighborhood $N(x)$ is defined as the set of states y that are adjacent to x, that is, the set of states that can be reached directly from x, taht is, with one move, or in a single step. The neighborhood size is $n(x) = |N(x)| \le n = \max_x n(x)$. We assume that the neighborhood structure is symmetric, that is, $y \in N(x) \Rightarrow x \in N(y)$, and that any two states, x and y, are linked by a path with at most m steps. Our aim is to minimize a finite and positive objective function, $H(x)$, with an unique global minimum attained at x^*. The system's Lipschitz constant, Δ, is the maximum difference in the value of H, for adjacent states, that is,

$$\Delta = \max_x \max_{y \in N(x)} |H(y) - H(x)| \ .$$

The Gibbs distribution is defined as

$$g(\theta)_x = \frac{n(x)}{Z(\theta)}\exp(-\theta H(x)) \ , \quad \text{with} \quad Z(\theta) = \sum_x n(x)\exp(-\theta H(x)) \ .$$

The Gibbs distribution specifies state probabilities in many systems of Statistical Physics, where the Hamiltonian function, H, represents state energies, and the parameter θ is the system's inverse temperature. The normalization constant, $Z(\theta)$, is called the partition function.

The Metropolis kernel is defined by

$$
P(\theta)_x^y = \begin{cases} \frac{1}{n(x)} \exp\left((H(x) - H(y))^+\right) , & \text{if } y \in N(x) \\ 1 - \sum_{y \in N(x)} P(\theta)_x^y & \text{if } y = x \\ 0 & \text{otherwise} \end{cases} .
$$

Theorem 9 (Metropolis sampling). The Gibbs distribution $g(\theta)$ is invariant for the metropolis kernel $P(\theta)$.

Proof. It suffices to prove the detailed balance equation

$$
g(\theta)_x P(\theta)_x^y = g(\theta)_y P(\theta)_y^x
$$

If $y \notin N(x)$, balance is trivial. Otherwise, we use

$$
\frac{1}{n(x)} \exp\left((H(x) - H(y))^+\right) = \frac{1}{n(x)} \left(\frac{g(\theta)_y n(x)}{g(\theta)_x n(y)} \wedge 1 \right) .
$$

Assuming that $(g(\theta)_y n(x))/(g(\theta)_x n(y)) \geq 1$,

$$
g(\theta)_x P(\theta)_x^y = \frac{g(\theta)_x}{n(x)} \quad \text{and } g(\theta)_y P(\theta)_y^x = \frac{g(\theta)_y}{n(y)} \frac{g(\theta)_x n(y)}{g(\theta)_y n(x)} = \frac{g(\theta)_x}{n(x)} .
$$

The case $(g(\theta)_y n(x))/(g(\theta)_x n(y)) < 1$ follows similarly.

We will now study an appropriate cooling schedule $\theta_1, \theta_2, \ldots$, for the Simplified Metropolis Algorithm where, at each temperature $1/\theta_t$, we take m steps using the kernel $P\{t\} = P(\theta_t)$, or a single step using the kernel $Q\{t\} = P\{t\}^m$

Theorem 10 (Logarithmic Cooling). In the simplified Metropolis algorithm, for any monotone decreasing cooling schedule

$$
\frac{1}{\theta_t} \geq \frac{\Delta m^2 \ln(n)}{\ln(t)}
$$

and any initial distribution w,

$$
\lim_{t \to \infty} \|wQ\{1\}Q\{2\} \ldots Q\{t\} - v\{\infty\}\| = 0 .
$$

Proof. From the definition of the system's Lipschitz constant, and from the fact that any two states of the system are conected by a path of lenght at most m, it follows that, for any two states, x and y,

$$
Q\{t\}_x^y \geq \left(\frac{1}{n} \exp\left(-\Delta\theta_t\right) \right)^m = \frac{1}{n^m} \exp\left(-m\Delta\theta_t\right) .
$$

Hence,

$$\rho\{t\} = \rho(Q\{t\}) = \max_{x,y}\left(1 - \sum_z \left(Q\{t\}_x^z \wedge Q\{t\}_y^z\right)\right) \le$$

$$\max_{x,y}\left(1 - \left(Q\{t\}_x^{z*} \wedge Q\{t\}_y^{z*}\right)\right) \le 1 - \frac{1}{n^m}\exp\left(-m\Delta\theta_t\right) =$$

$$1 - \frac{1}{n^m}\exp\left(-m\Delta\frac{\ln(t)}{\Delta m^2 \ln(n)}\right) = 1 - \frac{1}{n^m}\frac{n^m}{t} = 1 - \frac{1}{t}\ .$$

Condition (c) of the strong ergodicity lemma follows from

$$\sum_{t=1}^{\infty}\frac{1}{t} = \infty \;\Rightarrow\; \rho\{1::\infty\} = \prod_{t=1}^{\infty}\left(1 - \frac{1}{t}\right) = 0\ .$$

Finally, in orther to check condition (a) the strong ergodicity lemma, we must show that the invariant measures $v\{t\} = v(\theta_t)$ constitute a Cauchy sequence. However, as $\theta \to \infty$, the elements of $v\{t\}$ are either increasing for $x = x^*$ or decreasing for $x \ne x^*$ and sufficiently large θ. Hence, for $t \ge l$,

$$\sum_{t=l}^{\infty}\|v\{t+1\} - v\{t\}\| = \sum_{t=l}^{\infty}\sum_{x\in X}\left(v\{t+1\} - v\{t\}\right)^+ \le$$

$$\sum_{x\in X}\left(v\{\infty\} - v\{l\}\right)^+ < \infty\ .$$

There is an implicit choice of scale in the unit taken to measure the Hamiltonian or objective function, $H(x)$. An adequate scale should start the annealing process with a good acceptance rate for hill climbing moves. The step size of the logarithmic cooling schedule is inversely proportional to the *cooling constant*, $\Delta m^2 \ln(n)$. An alternative to the simplified Metroplis algorithm, taking m steps at each temperature θ_t, is to implement the standard Metropolis algorithm using the cooling constant $\Delta m^3 \ln(n)$.

H.3   Genetic Programming

The Intrinsic Parallelism Argument

Consider programs coded as binary (0-1) arrays of length n. A pattern or *schema* of *length l*, is a partial specification of a binary array of length l,

$$s[i] = 0, 1 \text{ or } * \text{ (don't-care)}\ ,\quad 1 \le i \le l\ .$$

The number of specified positions or *loci*, that is, l minus the number of don't-cares, defines the schema's *order*. The program's sub-array $p[j]$ in the *window* $k \le j \le k + l$, is an *instance* of schema s iff they coincide, in the specified loci, that is, iff $p[k + i] = s[i]$, for all $s[i] \ne *$.

The intrinsic parallelism argument, presented in chapter 6, requires an estimate of how many schemata of order l and length $2l$ can be represented in a program of length n.

Following Reeves (1991), consider the window of lenght $2l$ at the beginning or leftmost locus, $1 \leq j \leq 2l$, and let $B(2l, l)$ be the number of choices for the specified loci, l, among the $2l$ available positions. This first window can obviously represent $B(2l, l)\, 2^l$ distinct schemata, for once the l loci have been chosen, there are 2^l possible 0-1 attributions to their values.

Now slide the window $2l$ position to the right, so as to span positions $2l + 1 \leq j \leq 4l$. This new window has no positions in common with the previous one and can, therefore, represent the same number of schemata. If we keep sliding the window $2l$ position to the right until positions $n - 2l \leq j \leq n$ are spanned, it follows from Stirling's approximation that the total count of possible represented schemata, satisfies the relation

$$\frac{n}{2l} B(2l, l) 2^l \approx 2^{3l} \propto m^3 \ ,$$

where the population size is taken as $m = c\, 2^l$. The constant c is interpreted as the expected number of instances of any given schema (of order l and length $2l$) present in this population. Hence, under all the conditions above, we can (under) estimate the number of schemata present in the population as proportional to m^3. For generazations of the implicit parallelism theorem, see Bertoni, M.Dorigo (1993).

Stirling's Approximation

For large n,

$$\ln n! = \sum_{j=1}^{n} \ln j \approx \int_{j=1}^{n} \ln j\, dj = [j \ln j - j]_1^n = n \ln n - n + 1 \ .$$

A more detailed analysis of the remainder gives us

$$\ln n! \approx n \ln n - n + O(\ln n) \ .$$

From Stirling's approximation, the following Binomial approximations hold:

$$\ln \binom{n}{np} \approx nH(p) \ \text{ where } \ H(p) = -p \ln p - (1 - p) \ln(1 - p) \ .$$

$$\text{and } \ \ln \binom{2l}{l} \approx 2lH(1/2) \ .$$

H.4 Ontogenic Development

Autopoietic and alopoietic systems, living organisms and artificial machines, have both to be built up and have their basic components maintained. However, there are profound differences in their development processes. In this section we examine the structural similarities and differences between such systems, and how such structures can explain some properties of systemic development.

Herein, the adult or after construction systemic feature known as aging, receives special attention. Elementary or simple components have no structure, no internal states, and hence no memory. They can, therefore, exhibit no aging. Complex systems, however, exhibit some form of aging. We will see how the aging process of complex system can reflect systemic structure. We will contrast, in particular, bottom-up and top-down system construction, and their respective aging processes. Our analysis will follow Gavrilov (1981, 2001, 2006).

"The first fundamental feature of biosystems is that, in contrast to technical (artificial) devices which are constructed out of previously manufactured and tested components, organisms form themselves in ontogenesis through a process of self-assembly out of de novo forming and externally untested elements (cells). The second property of organisms is the extraordinary degree of miniaturization of their components (the microscopic dimensions of cells, as well as the molecular dimensions of information carriers like DNA and RNA), permitting the creation of a huge redundancy in the number of elements. Thus, we expect that for living organisms, in distinction to many technical (manufactured) devices, the reliability of the system is achieved not by the high initial quality of all the elements but by their huge numbers (redundancy)." Gavrilov (2001,p.531.)

Aging Processes

In this section we follow Gavrilov (1981, 2001, 2006) to analyse the aging process of some redundant series / parallel reliability systems.

As usual in reliability theory, t will denote failure time, $f(t)$ and $F(t)$ the density and cumulative distribution functions of the failure time, $S(t) = 1 - F(t)$ the survival function and

$$h(t) = \frac{d\,S(t)}{S(t)\,dt} = \frac{d\,\ln S(t)}{dt}$$

the hazard function, failure rate, or mortality force, see Barlow and Prochan (1981).

Simple, memoryless or non-aging components are characterized by exponentially distributed failure time. In this case, the failure time has constant hazard rate, $h(t) = \kappa$, and $S(t)) = \exp(-\kappa t)$, $\kappa, t \geq 0$. Complex systems are characterized by different aging regimes which, in turn, reflect their structural characteristics. Two aging regimes are of

special interest to us:

1- The Weibull or power law regime, with $h(t) = \kappa t^\alpha$, $\kappa, \alpha > 0$, characteristic of complex top-down, external assembly or alopoietic systems, and

2- The Gompertz-Mekeham regime, with $h(t) = A + R \exp(\alpha t)$, $A, R, \alpha > 0$, characteristic of complex bottom-up, self assembly or autopoietc systems. In biological models, the Mekeham parameter, A, indicates an external mortality force, whereas the pure Gompertz regime, for $A = 0$, models the internal or systemic hazard function.

In what follows, we will see some structural models that explain these two regimes and test them on some engineering and biological systems.

The two basic structures in reliability theory are parallel and series compositions. Complex systems in general, are recursive compositions of series and parallel blocks. A parallel block fails if all its components fail, whereas a series block fails if any one of its components fail, alternatively, a parallel block fails with its last failing component, whereas a series block fails with its first failing component. Hence the series-parallel reliability compositional rules:

- The cumulative distribution function of a parallel system with independent components equals the product of its components' cumulative distribution functions.

- The hazard function of a series system with independent components equals the sum of its components' hazard functions.

Let us now consider the "simplest complex system" modeling an organism or machine with multiple, m, functions, where each function is performed by an independent block of redundant simple components. That is, a system is assembled as a series of m blocks, $b_j, j = 1 \ldots m$, such that block j is assembled as a parallel (sub) system with n_j simple components.

Top-down projects typically use a small number of redundant units, in order to optimize production costs as well as to meet other project constraints such as maximum space or weight. Hence, components have to comply with strict standards, achieved by several forms of quality control tasks in the manufacturing process. In such systems all components are initially alive, operational or working, since they would have been otherwise rejected by quality control. They are typically depicted in block diagram of such as shown in Figure 1A. In this example each block has the same number, $n_j = i$, of redundant components.

Since each simple component has an exponential failure distribution, the reliability compositional rules lead to the following systemic hazard functions for each block,

$$F_j = \left(1 - e^{-\kappa t}\right)^i \ , \quad h_j(t) = \frac{i \kappa e^{-\kappa t} \left(1 - e^{-\kappa t}\right)^{i-1}}{1 - \left(1 - e^{-\kappa t}\right)^i} \ ;$$

and to the following systemic hazard function for the whole system,

$$h(t) = \sum_{j=1}^{m} h_j(t) = \frac{mi\kappa e^{-\kappa t}\left(1 - e^{-\kappa t}\right)^{i-1}}{1 - \left(1 - e^{-\kappa t}\right)^{i}} \ .$$

Using the early-life and late-life asymptotic approximations, $1 - \exp(-\kappa t) \approx \kappa t$, for $t << 1/\kappa$, and $1 - \exp(-\kappa t) \approx 1$, for $t >> 1/\kappa$, the i elements parallel block and systemic hazard functions can be approximated as

$$h_i(t) \approx \begin{cases} i\kappa^i t^{i-1} & \text{if } t << 1/\kappa \ \text{ and} \\ \kappa & \text{if } t >> 1/\kappa \ ; \end{cases} \ , \quad h(t) \approx \begin{cases} mi\kappa^i t^{i-1} & \text{if } t << 1/\kappa \ \text{ and} \\ m\kappa & \text{if } t >> 1/\kappa \ ; \end{cases} \ .$$

Let us now consider self-assembled blocks where the number i of initially working elements follows a Poisson distribution with parameter $\lambda = nq$, $P(i) = \exp(-\lambda)\lambda^i/i!$. We should also truncate the Poisson distribution, to account for the facts that the organism is initially alive, implying the exclusion of the $i = 0$ case, and that the organism is finite, implying a cut-off $\Pr(i > n) = 0$. The corrected normalization constant for this truncated Poisson is $c^{-1} = 1 - \exp(-\lambda) - \exp(-\lambda)\sum_{i=n+1}^{\infty} \lambda^i/i!$.

As in the previous model, the systemic hazard function is the sum of those of its blocks', where each block begins with i, Poisson distributed, working elements. Hence, the expected systemic hazard function can be written as:

$$h(t) = \sum_{j=1}^{m} h_j(t) = m \sum_{i=1}^{n} P(i)h_i(t) \ .$$

Substitution of $h_i(t)$ yields the following systemic hazard rate and approximations:

$$h(t) = cm\kappa\lambda e^{-\lambda}e^{-\kappa t}\sum_{i=1}^{n} \frac{\lambda^{i-1}\left(1 - e^{-\kappa t}\right)^{i-1}}{(i-1)!\left(1 - (1 - e^{-\kappa t})^{i}\right)} \ ,$$

$$h(t) \approx \begin{cases} cm\kappa\lambda e^{-\lambda}\sum_{i=1}^{n} \frac{(\kappa\lambda t)^{i-1}}{(i-1)!} = R\left(e^{\alpha t} - \epsilon(t)\right) & \text{if } t << 1/\kappa \ \text{ and} \\ m\kappa & \text{if } t >> 1/\kappa \ ; \end{cases} \ .$$

In the last expression, $R = cm\kappa\lambda\exp(-\lambda)$, $\alpha = \kappa\lambda$, and $\epsilon(t) = \sum_{i=n+1}^{\infty}(\kappa\lambda t)^{i-1}/(i-1)!$. For for fixed κ and λ and sufficiently small t, $\epsilon(t)$ is close to zero. Hence, in early life, $h(t) \approx R\exp(\alpha t)$, as in the pure Gompertz regime.

Appendix I

Research Projects

In the last courses we have had classes of very diverse students. As expected, we had students coming from the courses of Applied Mathematics, Physics and, of course, Statistics, but we also had some students with quite different backgrounds, such as Computer Science, Economics, Law, Logic and Philosophy. This appendix proposes some research projects that may be specially interesting to some of these students. I do believe, of course, that most of them will also be interesting to the student of Statistics. If you are interested in one of these projects, send me an e-mail, or stop by at my office, an let us talk about how to proceed.

Bayesian and other Credal Networks

The sparse factorization techniques described in Appendix F can be transposed to Bayesian Networks and other belief propagation networks as well.

1- Symbolic phase: Implement the algorithms used to find a good elimination order, like the Gibbs heuristics, the Bayes-ball algorithm, and the other graph algorithms mentioned in appendix F. A language such as C or $C++$, providing good support for dynamic data structures, is recommended.

2- Numeric phase: Once the elimination order, requisite variables, etc. are determined, implement the numerical elimination process using static data structures. A language such as Fortran, providing good support for automatic parallelization, is recommended.

3- Investigate the potential for parallelization of the sequential codes implemented in steps 1 and 2. Discuss the possibility, difficulties and advantages of developing tailor made parallel code versus the use of automatic parallelization tools.

4- Implement efficient MC or MCMC processes for computing the evidence supporting the existence of a given causal link, that is, the existence of a given arrow in (a) a given Bayes network topology (b) all or a given subset of topolgies.

Mixture of Factor Analyzers

Extend the theory and methods for Mixtures of Multivariate Gaussians, as described in appendix B, to Mixtures of FA's. The geometric interpretation of these models is very similar, but whereas all Mixtures of Gaussians lie in the same d-dimensional space, each Mixture of FA's lies in a different hyperplane of the full d-dimensional space. In particular:
a) Test the existence of a given component in the mixture.
b) Test the existence of the least significative dimension of a given component.

Polynomial Networks

1- Discuss the use of edge annotations and heuristic merit functions in the synthesis of sub-networks, that is, the use of heuristic "recombinative guidance", in the terminology of Nikolaev and Iba (2001, 2006).

2- Discuss the use of time dependent objective functions, as is section 5.2, to guide the synthesis of the entire network.

3- Discuss how to test (sub) topologies of a given network.

(De)Coupling, (De)Composition, Complementarity

1- Discuss the possibility of using complementary models in contexts other than Quantum Mechanics. Give examples of such applications.

2- Discuss the possibility of extending the results of Borges and Stern (2007) to models with limited dependence using, for example, the formalism of Copulas.

3- Investigate the meaning and interpretation of decoupling or separation schemes generated by alternative sparse and/or structured matrix factorizations.

4- Using wavelet or other self-similar representations, it is possible to overcome the strict version of Heisenberg uncertainty relation, see Vidakovic (1999, p.xxx). However, these representations may introduce non-local, delayed, integral, long-rage, long-memory or other forms of coupling or dependence. Investigate how to obtain generalized Heisenberg type relations for such cases.

5- Give suitable interpretations and implement statistical models for the "necessary or consequential randomness" implied in the following examples:

5a- Morgenstern and von Neumann (1947) and Nash (1951), proved the existence of equilibrium strategies for non-cooperative games. However, in general, these equilibria are not at deterministic or *pure* strategies, but at randomized or *mixed* strategies.

5b- The concept of Impossible (or Inconsistent, or Unholy) Trinity, also known as the Mundell-Fleming trilemma, is an hypothesis of international economics, stating the

impossibility of achieving simultaneously the follong goals: 1- fixed exchange rate; 2- free capital movement; and 3- independent monetary policy.

Economics

The economic system may be characterized by eigen-solutions, equilibria or fixed points resulting from the collective interaction of many economic agents. Some of the most important of such eigen-values are prices, see for example Ingrao and Israel (1990).

1- Give concrete examples of such situations, that are well suited for experimental research.

2- Discuss how to measure the epistemic value of such an economic or finacial eigen-value.

3- Discuss how to assess the consistency of such eigen-values, for example, by means of sensitivity analyses.

4- Discuss the need for regulatory mechanisms protecting such eigen-solutions such as, for example, anti-trust laws.

5- Discuss the consequences of Zangwill's global convergence theorem to the design of good regulatory policies; see, for example, Border (1989), Ingrao and Israel (1990) and Zangwill (1964).

Law

The Objective / Subjective dichotomy manifests itself in the legal arena via the notion of responsibility. Responsibility may require either two or three conditions, namely.

a) Damage: A loss suffered by the victim (or offended party).

b) Causal relation: A causal nexus linking an action (or lack thereof) of the accused (or defendant, offending party, perpetrator) to the damage suffered by the victim.

c) Illicitness: An explanation why the action (or lack thereof) of the accused was illegal or unlawful.

While the programs and codes (in Luhmann's sense) needed for checking condition (c) are internal ones, that is, programs and codes within the legal system itself, the programs and codes needed for checking conditions (a) and (b) are often external, that is, programs and codes of another systems, such as science or economics, for example.

Hence, it is not surprising that a responsibility entailed by conditions (a) and (b) alone is called "objective", while one requiring conditions (a), (b) and (c) is called "subjective", see Stern (2007).

R.B.Stern (2007) suggests the following principle, hereby named "Transference of Objectivity" (TrOb), for systems characterized by the existence of eigen-solutions resulting from complex collective interactions:

If an individual agent (or a small group of agents) in the system disrupts such an eigen-solution, hence destroying its objective character, then this agent becomes, in the same measure, objectively responsible for consequential damages caused by the disruption.

1- Discuss the plausibility of the TrOb principle.

2- Discuss possible justifications for the TrOb principle.

3- Discuss the applicability of the TrOb principle in:
a) Economic law; b) Environmental law.

5- Discuss the applicability of TrOb for state actions.

5- Discuss the applicability of TrOb for lost revenues.

6- Discuss the applicability of TrOb for the loss of a chance.

Experiment Design and Philosophy

1) Discuss the possibility of conciliating the objective inference entailed by randomization methods with biased allocation and selection procedures.

2) Discuss the possibility of using optimal selections or allocations obtained by Multi-Objective or Goal Programming, where some (fake or artificial) explaining variables have randomly generated values.

3) Discuss the possibility of using low-discrepancy selections or allocations obtained by quasi-random or hybrid (scrambled quasi-random) lattices.

4) How can we corroborate the objective character of such inference procedures? For example, what is the importance of sensitivity analyses in these allocation?

5) What kind of protocols are appropriate for such inference procedures?

6) What criteria can be used in balancing the epistemic value of a clinical study versus the well being of the participants? What kind of moral, ethical and legal arguments can be used to support these criteria?

Art

Make your contribution to the Art Gallery.

Appendix J

Image and Art Gallery

The images in this gallery are somehow related to topics discussed in the main text. They are provided with no fixed definite interpretation, and only meant as a stimulus to imagination and creativity. Paraphrasing an aphorism of the poet Fernando Pessoa,

 – *There is no good science that is vague, nor good art or poetry that is not.*

Additional contributions to the art gallery, many made by students or interested readers, can be found at `www.ime.usp.br/~jstern/books/gallery2.pdf`.

Figure JA.1: Wire Walking.
The most important thing is not to fear at all.

Figure JA.2: Ludwig Boltzmann, Cartoon by K.Przibram.
Moving ahead, no matter what.

Figure JA.3: Albert Einstein in his Bicycle.
Following the gentle curvature of the garden's geometry.

Figure JA.4: Niels Bohr in his Bicycle.
Complementary pedals must be pushed one at a time.

Figure JA.5: Empirical Science: All at Once!
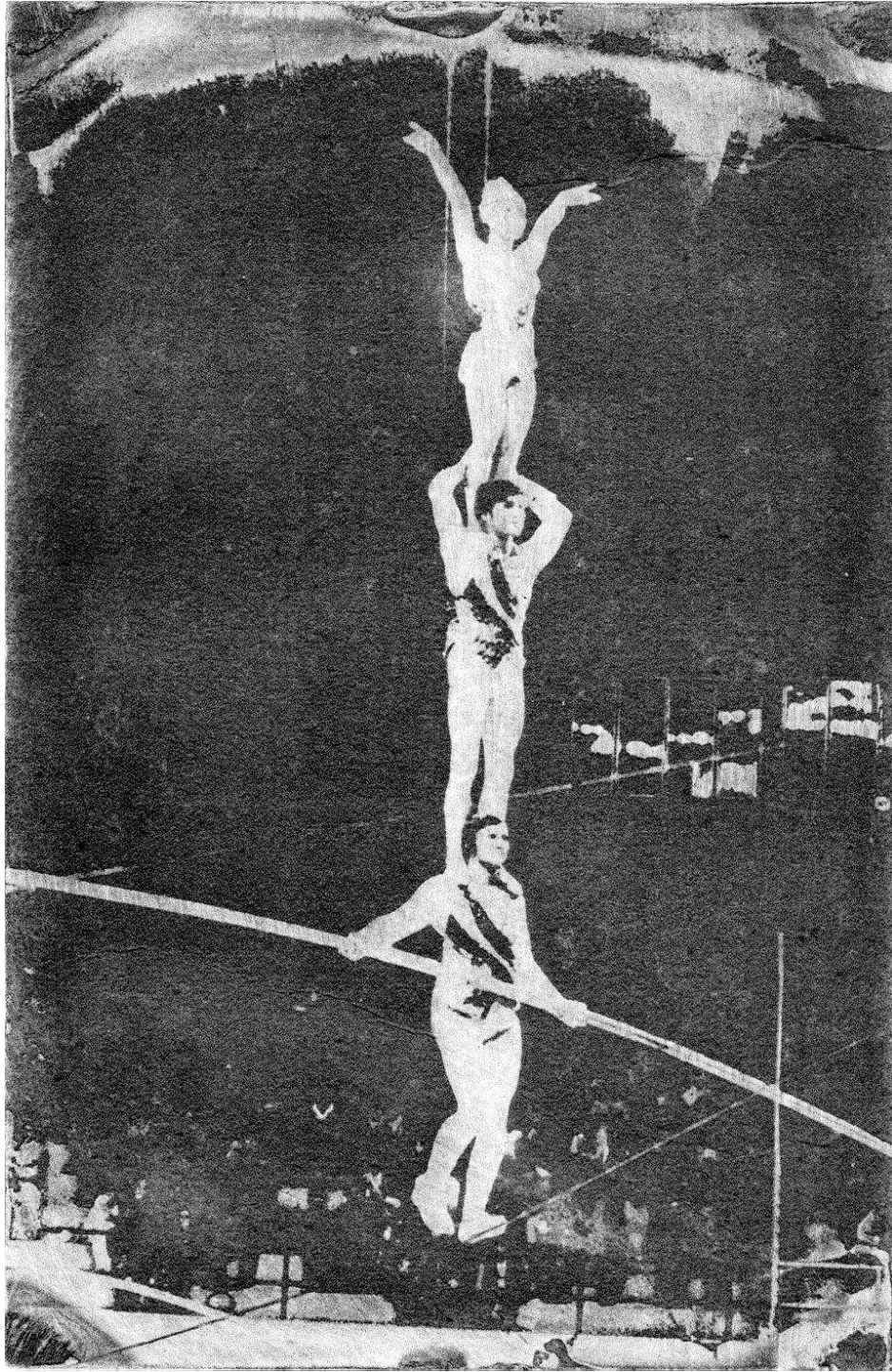Caution: Do this only at a fully equipped laboratory.

Figure JA.6: Triadic (or Semiotic) Wire Walking.
Etching by Alex Flemming (untitled, 1979, PA III/X),
based on a photo of the Moscow Circus at São Paulo.
Private collection of Marisa Bassi Stern.