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Covariance Realization Problem for Spin Systems

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Abstract

Let $(\Omega, \mathcal{A})$ be a measurable space, $\mathcal{F}$ be a family of measurable functions f from Ω to $\mathbb{R}$, and $c : \mathcal{F} \longrightarrow \mathbb{R}$ be a given function. A **generalized moment problem** consists of finding all probabilities P on $(\Omega, \mathcal{A})$ such that $\int f dP = c(f) = c_f$ for all $f \in \mathcal{F}$, and in providing conditions on $(c)_{f \in \mathcal{F}}$ for the existence of at least one such probability. Generalized moment problems of this kind have been widely studied, mainly in the theoretical engineering community, for continuous random variables.

In this thesis, we consider the special case of the **covariance realization problem** for spin systems and discuss the necessary and sufficient conditions for the realizability of a correlation matrix of order $n \geq 2$. Let $\Omega_n = \{-1, 1\}^n$ be the space of length-n sequences which are denoted by $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_n)$, where $\sigma_i \in \{-1, 1\}$. Define the spin random variables $\xi_i : \Omega_n \longrightarrow \{-1, 1\}$ for $1 \leq i \leq n$ as $\xi_i(\sigma) = \sigma_i$. For a probability P on Ω_n, we denote by E_P the expectation with respect to P. Given a symmetric matrix $C = ((c_{ij}))$, we ask the following question in this thesis: under what condition does there exist a probability P such that $E_P(\xi_i) = 0$ and $c_{ij} = E_P(\xi_i \xi_j)$ for $1 \leq i < j \leq n$. In this case, we say that C is a spin correlation matrix.

The necessary and sufficient conditions for a symmetric matrix of order $n \leq 4$ to be a spin correlation matrix are already known. In this thesis, we obtain a general set of inequalities that are necessary and sufficient for any n. We also give a minimal set of necessary and sufficient conditions for $n = 5, 6$. Finally, we discuss methods to explicitly find the measure that realizes the given spin correlations (if they are feasible). We give a deterministic algorithm as well as a stochastic version of the same algorithm to find the measure explicitly. The efficiency of different algorithms is compared and some examples are worked out to illustrate the point.

Sommario

Sia $(\Omega, \mathcal{A})$ uno spazio misurabile, $\mathcal{F}$ una famiglia di funzioni misurabili f da Ω a $\mathbb{R}$, e $c : \mathcal{F} \longrightarrow \mathbb{R}$ sia una funzione assegnata. Un **problema dei momenti generalizzato** consiste nel trovare tutte le probabilità P su $(\Omega, \mathcal{A})$ tali $\int f dP = c(f) = c_f$ per ogni $f \in \mathcal{F}$, e nel determinare le condizioni su $(c)_{f \in \mathcal{F}}$ per l'esistenza di almeno una tale probabilità. Problemi dei momenti generalizzati di questo tipo sono stati ampiamente studiati, principalmente dagli ingegneri teorici, per variabili casuali continue.

In questa tesi consideriamo il caso speciale del **problema di realizzazione della covarianza** per sistemi di spin e discutiamo le condizioni necessarie e sufficienti per la realizzabilità di una matrice di covarianza di ordine $n \geq 2$. Sia $\Omega_n = \{-1, 1\}^n$ lo spazio delle sequenze di lunghezza n, denotate con $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_n)$, dove $\sigma_i \in \{-1, 1\}$. Definiamo le variabili aleatorie di spin $\xi_i : \Omega_n \longrightarrow \{-1, 1\}$ per $1 \leq i \leq n$ ponendo $\xi_i(\sigma) = \sigma_i$. Data una probabilità P su Ω_n, denotiamo con E_P il valore atteso rispetto a P. Data una matrice simmetrica $C = ((c_{ij}))$, nella tesi ci poniamo la seguente domanda: sotto quali condizioni esiste una probabilità P tale che $E_P(\xi_i) = 0$ e $c_{ij} = E_P(\xi_i \xi_j)$ for $1 \leq i < j \leq n$? In questo caso, diciamo che C è una matrice di correlazione per spin.

Condizioni necessarie e sufficienti affinché una matrice simmetrica di ordine $n \leq 4$ sia una matrice di correlazione per spin sono note. In questa tesi forniamo una famiglia di disuguaglianze che costituiscono una condizione necessaria e sufficiente per ogni n. Inoltre, per $n = 5, 6$, forniamo l'insieme di condizioni necessarie e sufficienti minimali. Infine, discutiamo vari metodi per determinare una probabilità che realizza le correlazioni assegnate (se ne esiste almeno una). Forniamo per questo un algoritmo deterministico, e alcune versioni stocastiche dello stesso. Confrontiamo inoltre, su alcuni esempi, l'efficienza di tali algoritmi.

Introduction

Moment Problems

Moment Problems arise naturally in many areas of applied mathematics, statistics and probability, economics, engineering, physics and operations research. For example, how does one price derivative securities in a financial economics framework without assuming any model for the underlying price dynamics, given only moments of the price of the underlying asset? A generalized moment problem can be defined as follows:
Let $(E, \mathcal{E})$ be a measurable space and $\mathcal{F}$ be a set of measurable functions

$$f : E \longrightarrow \mathbb{C}$$

Given, $c_i = c(f_i) \in \mathbb{C}$ for $i \in \mathcal{I}$ (where $\mathcal{I}$ is some index set), the moment problem consists of two main questions:

1. Find a measure μ such that

$$\int_E f_i(t) d\mu(t) = c_i \qquad \text{for } \; i \in \mathcal{I}$$

2. Is μ uniquely determined by c_i.

The first part concerns itself with finding explicit necessary and sufficient conditions for existence of such a measure. One can associate interesting questions like whether the measure is continu-

ously dependent on the scalars c_i.

Historically moment problems came into focus in context of studying the analytic behavior of continued fractions. The origin and subsequent developments are discussed in much detail in the paper of Tinne Hoff Kjeldsen [19]. We present a short summary of it here to put the problem in perspective. For a considerable amount of time moment problems lurked behind as an essential ingredients in formulation of other important problems in analysis until they became an important independent set of problems.

The initial interest in these kind of problems in analysis dates back to 1874 when Chebyshev was working on a problem of how can one determine an upper (resp. lower) bound for $\int_a^b f(x)dx$, given the values of the integrals

$$\int_A^B x^k f(x)dx$$

(where $[a, b] \subset [A, B]$ and $k = 1, 2, \ldots, m$ for some m). He associated the problem with the expansion of the integral in a continued fraction. Later in 1894-1895, Thomas Jan Stieltjes formulated the moment problem on positive real axis and used it as a means of studying the analytic behavior of continued fractions, in which connection he invented the important Stieltjes integral. He was studying the relationship between definite integrals, infinite series, and continued fractions. It was already well known that one could transform an infinite series into a continued fraction and vice versa [Euler 1748]. Laguerre (1834-1886) came up with another interesting aspect of the relationship between definite integrals, infinite series, and continued fractions. While studying the integral $\int_x^\infty \frac{e^{-x}}{x}dx$, he obtained the following:

$$\int_x^\infty \frac{e^{-x}}{x}dx = e^{-x}F(x) \mp 1.2.3 \ldots n \int_x^\infty \frac{e^{-x}}{x+1}dx$$

where

$$F(x) = \frac{1}{x} - \frac{1}{x^2} + \frac{1.2}{x^3} - \frac{1.2.3}{x^4} + \ldots \pm \frac{1.2.3 \ldots (n-1)}{x^n}$$

If $F(x)$ is continued to an infinite series it will diverge for all values of x, but Laguerre pointed out that it is possible to transform $F(x)$ into a continued fraction which is convergent, thus, providing a plausible method to determine the value of the integral. Stieltjes was interested in this partic-

ular connection between the continued fractions and definite integrals and wanted to generalize Laguerre's observation. By the end of the 1880's Stieltjes expanded various definite integrals into continued fractions.

In 1919, Hamburger extended the "Stieltjes moment problem," which was only defined on the positive real axis, to the "Hamburger moment problem," which is defined on the whole real axis. This was the first profound and complete treatment of the moment problem. From being primarily a tool for the determination of convergence/divergence of continued fractions it now became established as an independent problem. In 1920, Hausdorff stated and solved the Moment problem on a bounded interval. This is called the Hausdorff Moment Problem.

Theorem 0.0.1. *(Hausdorff) A sequence* $\{c_i\}_{i\geq 0}, c_0 = 0$*, is the moment sequence of some probability measure on* $[0, 1]$ *if and only if it is completely monotone.*

where being completely monotone means that $(-1)^n \Delta^n c_k \geq 0$ (for $k, n = 0, 1, 2, \ldots$), where $\Delta c_k = c_{k+1} - c_k$ and Δ^n stands for n applications on Δ.

Moments problems are fairly common in spectral estimation, speech synthesis, system identification, image processing and there are some very interesting results in these areas recently. There are also interesting versions of Moment problems in Physics, for example, given a system of particles, it seems almost natural to ask for a possible probability distribution of particles given a measurable quantity representing their interactions is known. Covariance Realization Problem for spins is one such problem.

Spin Systems

Classical spin systems on a lattice are widely studied in statistical mechanics. The spin variables are theoretically idealized versions of magnetic orientation (or angular momentum vector of a spinning particle). Some of the most studied mathematical models for spins include the Ising model, the "XY" model (where the spin variables take values on a circle.), Curie-Weiss model etc. Of

course the most fitting model depends on the problem being considered. To start with, we need to know the degrees of freedom of the spin variables under consideration. Other than that, one is also concerned with where these spins are. That is, one may think of spins to represent particles at each point of some lattice in some dimension (which could be a very good model for certain many-body particle interaction problems in statistical mechanics), or they could be distributed continuously. The third important factor that shapes the possible mathematical model is the interaction between spins, that is, the energy associated with each particular conguration of spins. Two major types of interaction are called "ferromagnetic", where the energy is lowered when two spins are aligned (same signs), and "antiferromagnetic", where the energy is lowered when they point in opposite directions (opposite signs).

In this thesis we consider a covariance realization problem for spin systems. Covariance realizations are just a special case of Generalized Moment Problem where instead of moments of a random variable, we are given the correlations or the covariances between a set of random variables and we want to find a stochastic process that realizes these covariances. In other words, given a matrix $C = ((c_{ij}))$, we want to find random variables $X_1, X_2, \ldots, X_n$ such that $c_{ij} = Cov[X_i, X_j]$. The problem makes it important to understand the geometry of covariance matrices in general. The convex set of covariance matrices known as the Positive Semidefinite Cone has been studied in much detail. In 1998, Parathasarathy, gave a complete description of this set. His work has been discussed briefly in chapter 2. In this thesis, we deal with the case where the random variable X_i's are constrained to take values in $\{-1, 1\}$ and to have mean zero.

Covariance between two spins is essentially a measure of interaction of the two particles that these spin variables represent. This gives rise to many interesting questions. Two important questions addressed in this thesis are the following:

1. What are the necessary and sufficient conditions on c_{ij} so that $C = ((c_{ij}))$ is realized a covariance matrix of a spin system? In fact, we do not assume that all the c'_{ij}s are given. So, the covariance matrix is not necessarily complete.

2. If a given $C = ((c_{ij}))$ is known to satisfy the necessary and sufficient conditions, that is, if

it is realizable, how does one explicitly find a joint spin distribution that realizes it?

We consider the first problem in detail in chapter 3, while the second one is addressed in chapter 4. In chapter 5, we analyze some stochastic algorithms to solve the second problem. To make this thesis self-sufficient, we start with some basic background of convex analysis in chapter 1.

Chapter 1

Convex Analysis: Some Background

1.1 Basic Ideas

Convex analysis plays a very important role in the extremum problems in many areas in applied mathematics. It will be useful in dealing with extremum problem of correlation matrices in the particular context of this thesis. In this chapter, we will look at some of the basic concepts of convexity, duality between points and hyperplanes, different representations of the convex hull of a set S etc.

Let us consider $\mathbb{R}^n$ with the usual inner product, i.e., for $x, y \in \mathbb{R}^n$:

$$\langle x, y \rangle = \sum_{i=1}^{n} x_i y_i$$

Definition 1.1.1. A subset C of $\mathbb{R}^n$ is called convex if $(1-\alpha)x + \alpha y \in C$ whenever $x, y \in C$ and $0 < \alpha < 1$.

Definition 1.1.2. $\alpha_1 x_1 + \alpha_2 x_2 + \ldots + \alpha_n x_n$ is called a convex sum or a convex combination of $x_i's$ if $\alpha \geq 0$ for all $1 \leq i \leq n$ and $\alpha_1 + \ldots + \alpha_n = 1$.

Definition 1.1.3. The intersection of all convex sets containing A is called the *convex hull* of A and we will denote it by $\mathrm{conv}(A)$.

Below, we state some of the well-known facts about convex sets :

- Intersection of an arbitrary collection of convex sets is convex. (Hence, $\mathrm{conv}(A)$ defined above is convex)
- A subset of $\mathbb{R}^n$ is convex if and only if it contains all the convex combinations of its elements.

- For any $A \subset \mathbb{R}^n$, $\mathrm{conv}(A)$ consists of all the convex combinations of elements of A. In particular, the convex hull of a finite subset $\{b_0, b_1, \ldots, b_m\}$ of $\mathbb{R}^n$ consists of all the vectors of the form $\alpha_0 b_0 + \ldots \alpha_m b_m$, with $\alpha_i \geq 0$ for every $0 \leq i \leq m$ and $\alpha_0 + \ldots \alpha_m = 1$.

Definition 1.1.4. A subset K of $\mathbb{R}^n$ is called a cone if it is closed under positive scalar multiplication, i.e. $\alpha x \in K$ when $x \in K$ and $\alpha > 0$.

Definition 1.1.5. Convex conic sets. A set C is said to be **conic** if $x \in C$ implies $tx \in C$ for any $t \geq 0$. (It is easy to see that a conic set is convex if and only if $x_1, x_2 \in C$ implies that $x_1 + x_2 \in C$). A convex conic set which is not entire space is called a **wedge**. A closed wedge is called a **cone** if $x \in C$ and $-x \in C$ imply x = 0. A convex cone is **pointed** iff it contains no line.

Definition 1.1.6. Conic hull. The conic hull (resp. closed conic hull) of a set C is the intersection of all convex conic sets (resp. closed convex conic sets) containing C and is denotes by $\mathrm{cone}(C)$. The closed conic hull of C will be denoted by $\mathfrak{R}(C)$.

It is clear that given an arbitrary set C, $\mathrm{conv}(C) \subseteq \mathrm{cone}(C)$.

Definition 1.1.7. Give a vector $a = (\alpha_1, \ldots, \alpha_n)^T \in \mathbb{R}^n$ and a number h, the set of points x such that $\langle a, x \rangle = h$ is called a hyperplane.

Thus, a hyperplane in $\mathbb{R}$ is a point, a line in $\mathbb{R}^2$, a plane in $\mathbb{R}^3$, and so on.

Every hyperplane divides the entire space $\mathbb{R}^n$ into two open half-spaces (namely $\{x : \langle a, x \rangle > h\}$ and $\{x : \langle a, x \rangle < h\}$). The corresponding closed half-spaces are obtained by replacing strict inequalities by non-strict inequalities.

Theorem 1.1.1. *A closed convex set in $\mathbb{R}^n$ is equal to the intersection of all the half-spaces that contain it.*

A closed half-space is said to be a support of a set $A \subset \mathbb{R}$ if it contains A and its defining hyperplane contains at least one point of A. The hyperplane is called a support hyperplane.

Definition 1.1.8. An extreme point x of a convex set C is a point belonging to its closure $\overline{C}$ that is not expressible as a convex combination of point in $\overline{C}$ distinct from x.

A set P of $\mathbb{R}^n$ is called a convex polyhedron if it is the set of solutions of a finite system of linear inequalities, and called a convex polytope if it is a convex polyhedron and is bounded.
A nonempty closed convex set containing no lines has at least one extreme point.

Definition 1.1.9. A subset F of a polyhedron P is called a face of P if

$$F = P \cap \left\{x : c^T x = r\right\}$$

for some valid inequality $c^T x \leq r$.

We call the whole set and Φ as the improper faces. The faces of dimension $0, 1$ are called vertices and edges respectively. The 1-dimensional set $\{\gamma x + x_0 : \gamma \geq 0, x \neq 0\} \subset \mathbb{R}^n$ defines half-line called a *ray* in the non-zero direction $\{x \in \mathbb{R}^n\}$. Note that the vertices coincide with the extreme points of P.

Theorem 1.1.2. *The following properties of a convex set C are equivalent:*

1. *C is a polyhedral.*
2. *C is closed and has finitely many faces.*
3. *C is finitely generated.*

For a convex polyhedron P in $\mathbb{R}^n$, a real vector $c \in \mathbb{R}^n$ and a real number r, an inequality $c^T x \leq r$ is called valid for P if it holds for all $x \in P$.

In context of above definition of convex cones, we define extreme directions.

Definition 1.1.10. An extreme direction r of a pointed closed convex cone C is a vector corresponding to an edge that is a ray emanating from origin. an extreme direction in a pointed closed convex cone is the direction of a ray, called an *extreme ray*, that cannot be expressed as a conic combination of directions of any rays in the cone distinct from it. Clearly, an extreme direction is unique, up to positive scaling.

Corollary 1.1.3. *A polyhedral convex set has at most a finite number of extreme points and extreme directions.*

Proof. This follows from the fact that the extreme points and the extreme directions correspond to the 0-dimensional faces and half-lines respectively. □

Let us now consider a more general definition of the convex hull. We consider the convex hull of sets A which consists of both points and directions (points at infinity).
Let A_0 be the set of points of $\mathbb{R}^n$ and A_1 be a set of directions of $\mathbb{R}^n$, we define the convex hull $\mathrm{conv}(A)$ of $A = A_0 \cup A_1$ to be the smallest convex set C in $\mathbb{R}^n$ such that $A_0 \subset C$ and C recedes in all the directions in A_1. So,

$$C = \mathrm{conv}(A_0) + \mathrm{cone}(A_1)$$

where $\mathrm{cone}\ A_1$ is the convex cone generated by all the vectors whose directions belong to A_1

Theorem 1.1.4. ***Caratheodory's Theorem*** *Let S be any set of points and directions in $\mathcal{R}^n$ and let $C = \mathrm{conv}(S)$. Then $x \in C$ if and only if x can be expressed as the convex combination of $n+1$ points and directions in S (not necessarily distinct). In fact C is the union of all the generalized $d-$dimensional simplices whose vertices belong to S, where $d = dim\ C$.*

where by a generalized $m-$dimensional simplex, we mean a set which is the convex hull of $m+1$ affinely independent points and directions.

Corollary 1.1.5. *Let $\{C_i | i \in I\}$ be an arbitrary collection of convex sets in $\mathbb{R}^n$, and let C be the convex hull of the union of the collection, then every point in C can be expressed as a convex combination of $n+1$ or fewer affinely independent points, each belonging to a different C_i.*

Note that in general, the convex hull of a closed set need not be closed.

Theorem 1.1.6. *If A is a bounded set of points in $\mathbb{R}^n$, then $\overline{\mathrm{conv}(A)} = \mathrm{conv}(\overline{A})$. In particular, if A is closed and bounded, then $\mathrm{conv}(A)$ is closed and bounded.*

Proof. It is easy to see that

$$\overline{\text{conv}(A)} = \text{conv}(\overline{\text{conv}(A)}) \supset \text{conv}(\overline{A})$$

For the converse, consider the space X defined by the set of all vectors $(\alpha_0, \ldots, \alpha_n, x_0, \ldots, x_n) \in \mathbb{R}^{(n+1)^2}$, such that $x_i \in \overline{A} \subset \mathbb{R}^n$ and $\alpha_i \in \mathbb{R}$ with $\sum_{i=0}^{n} \alpha_i = 1$.
Then, the image of X under the continuous map $(\alpha_0, \ldots, \alpha_n, x_0, \ldots, x_n) \mapsto \alpha_0 x_0 + \ldots + \alpha_n x_n$ from $\mathbb{R}^{(n+1)^2}$ to $\mathbb{R}^n$ is $\text{conv}(\overline{A})$ by Caratheodory's theorem. If A is bounded in $\mathbb{R}^n$, X is closed and bounded in $\mathbb{R}^{(n+1)^2}$, hence the image of X is also closed and bounded. So,

$$\text{conv}(\overline{A}) = \overline{\text{conv}(\overline{A})} \supset \overline{\text{conv}(A)}$$

□

1.2 The convex hull problem

For a subset A of $\mathbb{R}^n$, the convex hull $\text{conv}(A)$ is defined as the smallest convex set in $\mathbb{R}^n$ containing A.
The convex hull computation means the determination of $\text{conv}(A)$ for a given finite set of n points $A = \{p_1, p_2, \ldots, p_n\}$ in $\mathbb{R}^n$.

Theorem 1.2.1. ***Minkowski-Weyl's Theorem.*** *For a subset P of $\mathbb{R}^n$, the following statements are equivalent:*

1. *P is a polyhedron, i.e., for some real (finite) matrix A and real vector b, $P = \{x : Ax \leq b\}$.*
2. *There are finite real vectors $v_1, v_2, \ldots, v_d$ and $r_1, r_2, \ldots, r_s$ in $\mathbb{R}^n$ such that $P = \text{conv}(v_1, v_2, \ldots v_d) + \text{nonneg}\ (r_1, r_2, \ldots, r_s)$, where nonneg denotes the non-negative hull of a finite set of points in R^n.*

Thus, every polyhedron has two representations of type (1) and (2), known as (Half-space) H-representation and (Vertex) V-representation, respectively.

1.2.1 The Vertex Enumeration problem and the Facet Enumeration problem

When a polyhedron P in $\mathbb{R}^n$ has at least one extreme point and is full dimensional, both representations (1) and (2) in Miknowski-Weyl Theorem are unique up to positive multiples of each inequality and ray r_j. Under these regularity conditions, the conversions between the H-representation and the V-representation are well-defined problems. The transformation (1) to (2) is known as the vertex enumeration and (2) to (1) is known as the facet enumeration.

Remark 1.2.1. If P a polytope, the facet enumeration problem reduces to the convex hull problem defined above.

Remark 1.2.2. If a given polyhedron does not satisfy the assumptions, it is easy to transform the polyhedron to an isomorphic lower dimensional polyhedron satisfying the assumptions.

One of the main questions considered in this thesis is that of Facet Enumeration Problem in context of Spin systems. We will discuss this problem in detail in chapter 3.

Chapter 2

Moments Problems and Correlation Matrices

2.1 Generalized Moment Problems

The Generalized moment Problems are of particular interest in linear optimization and can be stated as follows: Let $(E, \mathcal{E})$ be a measurable space and $\mathcal{F}$ be a set of measurable functions

$$f : E \longrightarrow \mathbb{C}$$

Given, $c_i = c(f_i) \in \mathbb{C}$ for $i \in \mathcal{I}$ (where $\mathcal{I}$ is some index set), the moment problem consists of two main questions:

1. Find a measure μ such that

$$\int_E f_i(t) d\mu(t) = c_i \qquad \text{for } \ i \in \mathcal{I}$$

2. Is μ uniquely determined by c_i.

If the measure is indeed uniquely determined by its moments, that is, if the answer to second question is yes then the moment problem is called determinate, otherwise it is called indeterminate.

The problem of determinateness/indeterminateness of moment problem is rather interesting. It is in fact easy to construct an example of an indeterminate moment problem, the most famous one being the following:

Example 1.

$$X \sim N(0, 1)$$

Let $Y = e^X$, then Y has what is called the log-normal distribution which is given by the density function

$$f(x) = \frac{1}{x\sqrt{2\pi}} \exp\left\{-\frac{1}{2}(\log x)^2\right\}$$

For $|a| \leq 1$, define $f_a(x) = (1 + a\sin(2\pi \log x))f(x)$. This is a density function with moments

$$\int_{-\infty}^{\infty} x^k f(x)$$

which are just the moments of $f(x)$ and do not depend on a and hence we see that the probability measure is not determined by its moments.

We now look at a special case of moment problems called the covariance realization problems.

2.2 Covariance Realization problem

Covariance Realization Problem: Covariance realization problem is a special case of Generalized Moment Problem and can be stated as follows:

Given a matrix $C = ((c_{ij}))$, find random variables $X_1, X_2, \ldots, X_n$ such that

$$c_{ij} = \mathrm{Cov}[X_i, X_j]$$

The idea is to find a joint distribution of $(X_1, X_2, \ldots, X_n)$ which realizes the given covariance matrix.

Covariance Realization Problems and Covariance Extension Problems have a long history going back to potential theory. It has been of more recent interest due to its interface with problems of in signal processing, speech processing and in stochastic realization theory. We will look at the Covariance Realization Problem for Spin Variable in detail in the next chapter but before that we will give a geometric and algebraic description of covariance matrices. These results are crucial to understand the approach taken in the subsequent chapters to obtain a similar description of covariance matrices for spins.

2.2.1 Positive Semidefinite Cone

Consider a vector of random variables $X = \{X_1, X_2, \ldots, X_n\}$ with μ as a joint probability distribution of X. We call $C = ((c_{ij}))_{n\times n}$ (where $c_{ij} = \mathrm{Cov}[X_i, X_j]$) the covariance matrix of X. We define the Correlations matrix as

$$corr_{ij} = \frac{\mathrm{Cov}[X_i, X_j]}{\sqrt{Var(X_i)Var(X_j)}}$$

Covariance matrices are necessarily symmetric and positive semi-definite.

Proposition 2.2.1. *Every symmetric positive semi-definite matrix is a covariance matrix.*

Proof. Let M be a $n \times n$ symmetric, positive semi-definite matrix then, by the spectral theorem we know that there exists a matrix $M^{1/2}$ whose square is M. Now consider a vector of mutually independent random variables $X = (X_1, X_2, \ldots, X_n)$ with unit variance so that the covariance matrix of X is an identity matrix. Then, the covariance matrix of $M^{1/2}X$ is given by M. □

Definition 2.2.1. The set of all symmetric positive semidefinite matrices of particular dimension m is called the positive semidefinite cone. It is clearly convex.

Where by dimension m, we mean the matrices of order $m \times m$. The space of symmetric positive semidefinite matrices (S_+^m) is well-studied in convex analysis.

$$\begin{aligned} S_+^m &= \{A \in S^m : A \geq 0\} \\ &= \{A \in S^m : y^T A y \geq 0 \; \forall \|y\| = 1\} \\ &= \bigcup_{\|y\|=1} \{A \in S^m : \langle yy^T, A \rangle \geq 0\} \\ &= \{A \in S_+^m : \text{ rank } A \leq M\} \end{aligned}$$

where S^m denotes the set of $m \times m$ symmetric matrices. The positive definite (full-rank) matrices comprise the interior of the cone.

We have seen that being symmetric and positive semi-definite is necessary and sufficient for a matrix to be a covariance matrix.

Remark 2.2.1. Every symmetric positive semi-definite matrix with 1's on the diagonal is a correlation matrix and vice versa. So to understand the geometry of the set of correlation matrices is equivalent to understanding the geometry of the set of covariance matrices.

Denote by $\mathcal{C}_n$ the set of all such nth order correlation matrices. $\mathcal{C}_n$ is a convex set in the $n(n-1)$-dimensional Euclidean space of all symmetric matrices of order n with 1 on the diagonal. We already have a description of this space in terms of hyperplanes (the condition of positive semi-definiteness).

2.2.2 Extremal Correlations

Let $\mathcal{E}_n \subset \mathcal{C}_n$ be the subset of extremals of the set of correlation matrices of order n. That is, $\mathcal{C} = \text{conv}(\mathcal{E}_n)$. What are the elements of $\mathcal{E}_n$? In 1998, K. R. Parthasarthy [27] gave a complete description of $\mathcal{E}_n$. We reproduce the theorem and the proof here.

One of the interesting and rather easy to understand observation about $\mathcal{E}_n$ is that elements of $\mathcal{E}_n$ cannot be nonsingular. If $M \in \mathcal{E}_n$ were non-singular, there would exist $\delta > 0$ such that $M - \varepsilon I$ is positive definite for all $0 \leq \varepsilon\delta$. It follows that for any symmetric matrix $A \neq 0$ with all diagonal entries equal to 0, there exists $\varepsilon > 0$ such that both $M \pm \varepsilon A$ are positive definite and hence correlation matrices. Then, $R = \frac{1}{2}(M + \varepsilon A) + \frac{1}{2}(M - \varepsilon A)$ but this contradicts the extremality of M. The main theorem that characterizes the elements of $\mathcal{E}_n$ is as follows:

Theorem 2.2.1. *(K. R. Parthasarathy) Let R be an nth order correlation matrix of rank k. Then $R \in \mathcal{E}_n$ if and only if it admits the representation*

$$\left(\begin{array}{c|c} \Sigma & \Sigma A \\ \hline A'\Sigma & A'\Sigma A \end{array}\right) P^{-1} \tag{2.2.1}$$

where P is a permutation matrix of order n, Σ is a nonsingular correlation matrix of order k and A is a $k \times (n-k)$ matrix of the form $A = (\boldsymbol{a}^1, \boldsymbol{a}^2, \ldots, \boldsymbol{a}^{n-k})$, where $\boldsymbol{a}^i; (i = 1, 2, \ldots, (n-k))$ are column vectors of order k satisfying the following:

1. *$\boldsymbol{a}^{i'} \Sigma \boldsymbol{a}^i = 1$ for every i.*
2. *the rank of the set $\{\boldsymbol{a}^i \odot \boldsymbol{a}^i = 1, i = 1, 2, \ldots, (n-k)\}$ is $\binom{k}{2}$ where $\odot$ is defined as:*

$$\boldsymbol{a} \odot \boldsymbol{a} = (a_1 a_2, a_1 a_3, \ldots, a_1 a_k, a_2 a_3, \ldots, a_{k-1} a_k)$$

Proof. Let $R = ((\rho_{ij}))$ be an nth order correlation matrix of rank k. Then there exist unit vectors $u^1, u^2, \ldots, u^n$ such that

$$\rho_{ij} = \langle u^i, u^j \rangle = u^{i'} u^j$$

Since rank $R = k (\leq n)$ we can select indices $1 \leq i_1 < i_2 < \ldots < i_k \leq n$ such that $u^{i_1}, u^{i_2}, \ldots u^{i_k}$ are linearly independent and any $u^j (j \neq i_m \text{for} m = 1, \ldots, k)$ can be expressed as linear combination of these k vectors. Through an appropriate permutation σ of the set $\{1, 2, \ldots, n\}$ we may assume, without loss of generality, that $i_r = r, r = 1, 2, \ldots, k$. If the matrix of σ is also denoted by σ, it follows that

$$\sigma^{-1} R \sigma = \left(\begin{array}{c|c} \Sigma & \Sigma A \\ \hline A'\Sigma & A'\Sigma A \end{array}\right) \tag{2.2.2}$$

where,

$$\begin{aligned} &\Sigma = ((\langle u^i, u^j \rangle))_{1 \leq i,j \leq k} \\ &u^1, u^2 \ldots u^k \text{ are linearly independent,} \\ &u^{k+r} = a_1^r u^1 + a_2^r u^2 + \ldots + a_k^r u^k, \quad r = 1, 2, \ldots, n-k, \\ &A = (a^1, a^2, \ldots, a^{n-k}), \\ &a^{r'} = (a_1^r, a_2^r, \ldots, a_k^r). \end{aligned}$$

In particular, $a^{r'} \Sigma a^r = 1$ for every r. Taking σ to the right hand side of (2.2.2), we get the representation (3) with the condition (i) fulfilled. Note that R is extremal if and only if $\sigma^{-1} R \sigma$ is extremal for some permutation σ. So we shall assume that R has the form

$$R = \left(\begin{array}{c|c} \Sigma & \Sigma A \\ \hline A'\Sigma & A'\Sigma A \end{array}\right) = ((\langle u^i, u^j \rangle)) \tag{2.2.3}$$

where A, u^i are as defined above, and $u^1, u^2 \ldots u^k$ are linearly independent. Now we shall prove that the condition (ii) of the theorem is necessary for the extremality of R. Suppose that the

linear span of $\{a^i \odot a^i, 1 \leq i < j \leq n-k\}$ has dimension $< \binom{k}{2}$. Then there exist real numbers $\{\alpha_{ij}, 1 \leq i < j \leq k\}$ such that $\alpha_{ij} \neq 0$ for some $i < j$ and

$$\sum_{1 \leq r < s \leq k} a_r^i a_r^s \alpha_{rs} = 0 \text{ for every } i = 1, 2, \ldots, (n-k) \tag{2.2.4}$$

Now, consider the symmetric matrix,

$$H = \begin{bmatrix} 0 & \alpha_{12} & \alpha_{13} & \ldots & \alpha_{1k} \\ \alpha_{21} & 0 & \alpha_{23} & \ldots & \alpha_{2k} \\ \ldots & \ldots & \ldots & \ldots & 0 \\ \alpha_{k1} & \alpha_{k2} & \ldots & \alpha_{kk-1} & 0 \end{bmatrix}$$

where $\alpha_{ij} = \alpha_{ji}$. Since Σ is non-singular and positive definite its least eigenvalue, say λ_0 is strictly positive. Hence $\Sigma \geq \lambda_0 I_k$. We have,

$$|H| \leq \|H\| I_k \leq \lambda_0^{-1} \|H\| \Sigma$$

In particular, $\Sigma \pm \varepsilon H \geq 0$ for all $0 \leq \varepsilon \leq \lambda_0 \|H\|^{-1}$. Thus there exists $\varepsilon > 0$ such that both the matrices $\Sigma \pm \varepsilon H$ are strictly positive definite. Now the matrix R can be expressed as $R = \frac{1}{2}(R_+ + R_-)$ where,

$$R_\pm = \left(\begin{array}{c|c} \Sigma \pm \varepsilon H & (\Sigma \pm \varepsilon H)A \\ \hline A'(\Sigma \pm \varepsilon H) & A'(\Sigma \pm \varepsilon H)A \end{array} \right)$$

$$= \begin{pmatrix} I_k \\ \hline A' \end{pmatrix} (\Sigma \pm \varepsilon H) \left(\begin{array}{c|c} I_k & A \end{array} \right)$$

$R_\pm$ are correlation matrices and $R_+ \neq R_-$. This contradicts the extremality of R and hence completes the proof of necessity.

Now, we shall prove the sufficiency by showing that R is extremal under the conditions (i) and (ii) of the theorem. Let $R = pR_1 + (1-p)R_2$ for some $0 < p < 1$ and $R_1, R_2 \in \mathfrak{C}_n$. Choose $0 < \alpha < \min(p, 1-p)$ and write

$$\begin{aligned} R &= \frac{1}{2}\{[(p-\alpha)R_1 + (q+\alpha)R_2] + [(p+\alpha)R_1 + (q-\alpha)R_2]\} \\ &= \frac{1}{2}(S_1 + S_2) \end{aligned} \tag{2.2.5}$$

where $S_1 = R + \alpha K, S_2 = R - \alpha K$ are correlation matrices, $q = 1-p$ and $K = R_2 - R_1$. There

exist unit vectors $u^1, u^2, \ldots, u^n; v^1, v^2, \ldots, v^n; w^1, w^2, \ldots, w^n$ in $\mathbb{R}^n$ such that

$$\begin{aligned} R &= ((\langle u^i, u^j \rangle)) \\ S_1 &= ((\langle v^i, v^j \rangle)) \\ S_2 &= ((\langle w^i, w^j \rangle)) \end{aligned} \tag{2.2.6}$$

and $u^1, u^2 \ldots u^k$ are linearly independent. Let $e, f \in \mathbb{R}^2$ be unit vector such that $\langle e, f \rangle = 0$. Put

$$\xi^i = 2^{-1/2}(e \otimes v^i + f \otimes w^i), \tag{2.2.7}$$

where $\otimes$ denotes tensor product. Then, we have

$$\langle \xi^i, \xi^j \rangle = \frac{1}{2}(\langle v^i, v^j \rangle + \langle w^i, w^j \rangle) = \langle u^i, u^j \rangle, \;\; 1 \leq i, j \leq n$$

Thus, the correspondence $\xi^i \to u^i$ is scalar product preserving and there exists a linear isometry L such that $Lu^i = \xi^i$ for every i. Since

$$u^{k+r} = a_1^r u^1 + a_2^r u^2 + \ldots + a_k^r u^k, \;\; 1 \leq r \leq n - k$$

It follows that $\xi^1, \xi^2, \ldots, \xi^k$ are also linearly independent and

$$\left(\begin{array}{c|c} \Sigma + \alpha K_! & (\Sigma + \alpha K_1)A \\ \hline A'(\Sigma + \alpha K_1) & A'(\Sigma \pm \epsilon H)A \end{array} \right) \xi^{k+r} = a_1^r \xi^1 + a_2^r \xi^2 + \ldots + a_k^r \xi^k$$

By, (2.2.6), we conclude that,

$$e \otimes \left(v^{k+r} - \sum_{j=1}^{k} a_j^r v^j \right) + f \otimes \left(w^{k+r} - \sum_{j=1}^{k} a_j^r v^j \right) = 0$$

for $1 \leq r \leq n - k$. Since $\langle e, f \rangle = 0$ we have,

$$v^{k+r} = \sum_{j=1}^{k} a_j^r v^j \quad \text{and} \quad w^{k+r} = \sum_{j=1}^{k} a_j^r w^j$$

for $1 \leq r \leq n - k$. Using (2.2.3), (2.2.5), (2.2.6) and the above two relations we have,

$$\begin{aligned} \Sigma &= ((\langle u^i, u^j \rangle)) \;\; 1 \leq i, j \leq k \\ \Sigma + \alpha K_1 &= ((\langle v^i, v^j \rangle)) \;\; 1 \leq i, j \leq k \\ \Sigma - \alpha K_1 &= ((\langle w^i, w^j \rangle)) \;\; 1 \leq i, j \leq k \end{aligned}$$

where K_1 denotes the first $k \times k$ principal block in $K = R_2 - R_1$. Furthermore,

$$S_1 = \left(\begin{array}{c|c} \Sigma + \alpha K_1 & (\Sigma + \alpha K_1)A \\ \hline A'(\Sigma + \alpha K_1) & A'(\Sigma + \alpha K_1)A \end{array} \right)$$

$$S_2 = \left(\begin{array}{c|c} \Sigma - \alpha K_1 & (\Sigma - \alpha K_1)A \\ \hline A'(\Sigma - \alpha K_1) & A'(\Sigma - \alpha K_1)A \end{array} \right)$$

Note that the diagonal entries of K and hence of K_1 are zero. By (2.2.4) and the condition (i) of the theorem the diagonal entries of $A'K_1A$ are 0. If $K_1 = ((\beta_{rs}))$ then $\beta_{rr} = 0$ and

$$\sum_{r<s} a_r^i a_r^s \beta_{rs} = 0$$

By condition (ii) of the theorem, $\beta_{rs} = 0$ for all $1 \leq r < s \leq k$ and hence $K_1 = 0$. Thus $S_1 = S_2 = R$. So, $K = 0$ and $R_1 = R_2$. This shows that R is extremal. □

Remark 2.2.2. Note that the condition (2) of the theorem implies that $n - k \geq \binom{k}{2}$, shows that for a correlation matrix of order n and rank k to be an element of $\mathcal{E}_n$ it is necessary that $n \geq k(k+1)/2$. This result (the convex set of all the nth order correlation matrices contains an extreme point of rank k if and only if $n \geq k(k+1)/2$) was first proved by Grome et al. in 1990. It however, follows as a simple corollary of the above result.

As mentioned before, there has been a lot of work on covariance realization problems for certain processes because of the applications in electrical engineering and other fields. In 2010, T. Kuna, J. L. Lebowitz and E. R. Speer [21] gave necessary and sufficient conditions for realizability of pair correlations for point processes. A point process in a set X is a random collection of points in X, whose distribution is described by a probability measure μ on the set of all possible point collections. We are going to look at a special case of point processes in this thesis.

In the next chapter, we consider the covariance realization problem for spins and try to solve the problem using simple computational procedures, the so called maximum entropy solution, and understand the Vertex/Facet enumeration problem in this case.

We have seen that it is rather easy to check whether a given matrix is a correlation matrix or not (namely, by using the conditions of symmetry and positive definiteness). It turns out that even though the set of spin correlations is much smaller, the H-representation of the convex set is not easy to obtain. On the other hand, the V-representation of spin correlations is much simpler than that of general correlation matrices.

Chapter 3

Spin Systems

3.1 Covariance Realization Problem for Spin Systems

Let $\Omega_n = \{-1, 1\}^n$ be the space of length-n sequences which are denoted by $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_n)$, where $\sigma_i \in \{-1, 1\}$. Define the spin random variables $\xi_i : \Omega_n \longrightarrow \{-1, 1\}$ for $1 \leq i \leq n$ as follows:

$$\xi_i(\sigma) = \sigma_i$$

By abuse of notation, we denote the random variable ξ_i by its value σ_i. The space Ω_n with random variables ξ_i is referred to as a spin system.

We consider a probability on Ω_n and suppose that we are given the spin-spin correlations, $c_{ij} := E(\sigma_i \sigma_j)$ with respect to this probability (we assume $E(\sigma_i) \equiv 0$ for all $1 \leq i \leq n$), under what conditions does a distribution with those correlations exist, and how does one determine it? We are not assuming that all the $c_{ij}'s$ are given.

As we have seen above, the structure of correlation matrices is known. The spin correlations of order n being a subset of the correlation matrices of order n, lie inside the convex hull of all correlation matrices. It is a small subset of $\mathcal{C}_n$ and we will denote it by Cov_n. Even though the set of spin correlations is much smaller in comparison, the structure/description of it in terms of extremals (V-representation) or in terms of faces (H-representation) is far from obvious. We will discuss the existing results on the same and provide a way to obtain the H-representation for spin correlations (as we shall see, a complete V-representation is already known and is rather simple compared to the V-representation of all the correlation matrices that we saw in the previous chapter).

3.1.1 Bell's inequalities

$(\sigma_1, \sigma_2, \ldots, \sigma_n)$ be n spins (i.e. $\sigma_i = \pm 1$), with $E(\sigma_i) = 0$ for every i and $c_{ij} = E(\sigma_i \sigma_j)$, so that $c_{ii} = 1$ for every i. Then the famous Bell's inequalities (Bell, 1964) are defined as follows:

$$1 + \varepsilon_i \varepsilon_j c_{ij} + \varepsilon_j \varepsilon_k c_{jk} + \varepsilon_k \varepsilon_i c_{ki} \geq 0 \qquad \forall\, i < j < k \leq n \tag{3.1.1}$$

where $\varepsilon_s \,\epsilon\, \{-1, 1\}$ for all $1 \leq s \leq n$.

Why are Bell's inequalities important in this context? There has been much discussion over the years on Bell's theorem [3] (or Bell's inequalities) for Quantum spins. In a complete classical setting as above, it turns out that Bell's inequalities play a very important role in understanding the structure of Cov_n (especially for small n).

Theorem 3.1.1. *Bell's inequalities are necessary for a correlation matrix $C = ((c_{ij}))$ to be a spin correlation matrix.*

Proof. Let $C = ((c_{ij}))$ be a correlation matrix under a probability P on Ω_n. Then, $E_P(\sigma_i) = 0$ and $E_P(\sigma_i \sigma_j) = c_{ij}$. Note that, for any distinct $1 \leq i, j, k \leq n$:

$$(\varepsilon_i \sigma_i + \varepsilon_j \sigma_j + \varepsilon_k \sigma_k)^2 \geq 1$$

where ε's are as defined in (3.1.1). Then, we get

$$\begin{aligned} E_P[(\varepsilon_i \sigma_i + \varepsilon_j \sigma_j + \varepsilon_k \sigma_k)^2] &\geq 1 \\ 3 + 2(\varepsilon_i \varepsilon_j c_{ij} + \varepsilon_j \varepsilon_k c_{jk} + \varepsilon_k \varepsilon_i c_{ki}) &\geq 1 \\ 1 + \varepsilon_i \varepsilon_j c_{ij} + \varepsilon_j \varepsilon_k c_{jk} + \varepsilon_k \varepsilon_i c_{ki} &\geq 0 \end{aligned}$$

which are the Bell's inequalities. Thus, any spin correlation matrix must satisfy the Bell's inequalities. □

Since, $\mathrm{Cov}_n \subset \mathcal{C}_n$, there are matrices that are symmetric and positive semi-definite but do not satisfy the Bell's inequalities. In other words, there are matrices that are correlation matrices but are not spin correlation matrices. We look at one such example.

Example 2. *Consider a symmetric matrix*

$$C = \begin{pmatrix} 1 & c_1 & c_2 \\ c_1 & 1 & c_1 \\ c_2 & c_1 & 1 \end{pmatrix}$$

with $-1 \leq c_1, c_2 \leq 1$. Then, the condition for positive semi-definiteness is

$$1 - 2c_1^2 + c_2 \geq 0$$

and the Bell's inequalities are given by

$$1 \pm 2c_1 + c_2 \geq 0$$

For $c_1 \in (-\frac{1}{\sqrt{2}}, -\frac{1}{2}) \cup (\frac{1}{2}, \frac{1}{\sqrt{2}})$ and $c_2 = 0$, we get a matrix C that is symmetric and positive semi-definite, hence a correlation matrix but it doesn't satisfy the Bell's inequalities, so it can't be a spin correlation matrix.

Theorem 3.1.2. *(Balasubramanian, Gupta and Parthasarathy, 1998 [18])*
Bells inequalities are necessary and sufficient for a correlation matrix of order ≤ 4 to be the correlation matrix of spin random variables.

We have already seen (Theorem 3.1.1), that the Bell's inequalities are necessary. The above theorem is proved in two parts: first for $n = 3$ and then for $n = 4$ (It is trivial for $n = 2$). We will reproduce the proof for $n = 3$ and another crucial result here for the sake of completion. The proof for the case $n = 4$ is essentially the same and one can have a look at the original paper for details. Before we proceed to the proof, let us establish some facts and notations.

For $S \subset \{1, 2, \ldots, n\}$, define:

$$p_S = P(\{\sigma_i = -1 \; \forall \; i \in S, \sigma_j = 1 \; \forall \; j \notin S\})$$

Then, the multiple correlation map $\tau : S \longrightarrow \tau_S$ from subsets of $\{1, 2, \ldots, n\}$ into $[-1, 1]$ is defined as

$$\tau_S = \begin{cases} \mathbb{E}\left(\prod_{i \in S} \sigma_i\right) & \text{if } \; S \neq \phi \\ 1 & \text{otherwise} \end{cases} \tag{3.1.2}$$

Proposition 3.1.1. *Let $\tau : S \longrightarrow \tau_S$ be a map from the space of all subsets of $\{1, 2, \ldots, n\}$ into the closed interval $[-1, 1]$ such that $\tau_\phi = 1, \tau_{\{i\}} = 0 \; \forall \; i$. Then τ is a multiple correlation map of n spin variables if and only if*

$$\sum_{S \subset \{1,2,\ldots,n\}} (-1)^{|S \cap T|} \tau_S \geq 0 \quad \forall \quad T \subset \{1, 2, \ldots, n\}$$

Proof. By definition of τ_S, it follows that

$$\tau_S = \sum_{T \subset \{1,2,\ldots,n\}} (-1)^{|S \cap T|} p_T \tag{3.1.3}$$

Note that $(((-1)^{|S \cap T|}))$ is a $2^n \times 2^n$ orthogonal matrix. This implies,

$$p_T = 2^{-n} \sum_{S \subset \{1,2,\ldots,n\}} (-1)^{|S \cap T|} \tau_S \tag{3.1.4}$$

which must be positive for all T. Hence,

$$\sum_{S\subset\{1,2,\ldots,n\}} (-1)^{|S\cap T|}\tau_S \geq 0 \quad \forall \quad T \subset \{1,2,\ldots,n\} \tag{3.1.5}$$

Conversely, if we have the inequalities,

$$\sum_{S\subset\{1,2,\ldots,n\}} (-1)^{|S\cap T|}\tau_S \geq 0 \quad \forall \quad T \subset \{1,2,\ldots,n\}$$

We define the P_T by (3.1.4). Since by definition $\tau_\phi = 1$, from (3.1.3), we get that $\sum_T P_T = 1$. τ_S is then a multiple correlation map under the probabilities P_T. □

Theorem 3.1.3. *Let $C = ((c_{ij})), 1 \leq i, j \leq 3$ be a real symmetric matrix with $c_{ii} = 1\ \forall\ i$. Then C is the correlation matrix of three spin variables if and only if*

$$\begin{aligned}&\min\{1 + c_{12} + c_{23} + c_{31}, 1 - c_{12} + c_{23} - c_{31},\\ &1 - c_{12} - c_{23} + c_{31}, 1 + c_{12} - c_{23} - c_{31}\} \geq 0\end{aligned} \tag{3.1.6}$$

Proof. We already know that the Bell's inequalities are necessary.
For the proof of sufficiency, choose any real number δ such that $|\delta|$ does not exceed the left hand side of the inequality (3.1.6) Define the map $S \longrightarrow c_S$ on the space of subsets of $\{1,2,3\}$ by

$$c_\phi = 1, c_{\{i\}} = 0, c_{\{i,j\}} = c_{ij}(i \neq j), c_{\{1,2,3\}} = \delta$$

Let $q_T = \sum_{S\subset\{1,2,3\}} (-1)^{|S\cap T|} c_S$. Then, by the choice of δ we have

$$\begin{aligned}q_\phi &= 1 + c_{12} + c_{23} + c_{31} + \delta \geq 0\\ q_{\{1\}} &= 1 - c_{12} - c_{13} + c_{23} - \delta \geq 0\\ q_{\{2\}} &= 1 - c_{12} - c_{23} + c_{31} - \delta \geq 0\\ q_{\{3\}} &= 1 + c_{12} - c_{13} - c_{23} - \delta \geq 0\\ q_{\{1,2\}} &= 1 + c_{12} - c_{13} - c_{23} + \delta \geq 0\\ q_{\{2,3\}} &= 1 - c_{12} - c_{13} + c_{23} + \delta \geq 0\\ q_{\{1,3\}} &= 1 - c_{12} + c_{23} - c_{23} + \delta \geq 0\\ q_{\{1,2,3\}} &= 1 + c_{12} + c_{23} + c_{31} - \delta \geq 0\end{aligned}$$

Now sufficiency is immediate from proposition 3.1.1. □

Proposition 3.1.2. *Let $\tau : S \longrightarrow \tau_S, S \subset \{1,2,\ldots,n\}$ be a multiple correlation map of n spin variables. Define $\tilde{\tau} : S \mapsto \tilde{\tau}_S$ by*

$$\tilde{\tau}_S = \begin{cases}\tau_S & \text{if } |S| \text{ is even}\\ 0 & \text{if } |S| \text{ is odd}\end{cases}$$

Then $\tilde{\tau}$ is also a multiple correlation map for a family of n spin variables.

Proof. For any $T \subset \{1, 2, \ldots, n\}$ denote by T^c its complement. By proposition 3.1.1 we have

$$\sum_{|S| \ odd} (-1)^{|S \cap T|} \tau_S + \sum_{|S| \ even} (-1)^{|S \cap T|} \tau_S \geq 0$$
$$\sum_{|S| \ odd} (-1)^{|S \cap T^c|} \tau_S + \sum_{|S| \ even} (-1)^{|S \cap T^c|} \tau_S \geq 0$$

Adding these two and using the relation $|S| = |S \cap T| + |S \cap T^c|$ we get

$$\sum_{|S| \ even} (-1)^{|S \cap T|} \tau_S \geq 0$$

or, equivalently

$$\sum_S (-1)^{|S \cap T|} \tilde{\tau}_S \geq 0$$

The required result is now immediate from proposition 3.1.1.

□

Theorem 3.1.4. *Let $C = ((c_{ij})), 1 \leq i, j \leq 4$ be a real symmetric matrix with $c_{ii} = 1 \ \forall \ i$. Then C is the correlation matrix of four spin variables if and only if*

$$\begin{aligned} &\min\{1 + c_{ij} + c_{jk} + c_{ki}, 1 - c_{ij} + c_{jk} - c_{ki}, \\ &1 - c_{ij} - c_{jk} + c_{ki}, 1 + c_{ij} - c_{jk} - c_{ki}\} \geq 0 \end{aligned} \tag{3.1.7}$$

for any $1 \leq i < j < k \leq 4$.

The proof of the above theorem involves the same idea of constructing a multiple correlation map. Necessity is immediate from theorem 3.1.6. To prove the sufficiency it is enough to show the existence of a multiple correlation map $c : S \longrightarrow c_S, S \subset \{1, 2, \ldots, n\}$ for which $c_\phi = 1, c_S = 0$ when S is odd (from proposition 3.1.2), $c_{\{i,j\}} = c_{ij}$ for $i \neq j$ and $c_{\{1,2,3,4\}} = \delta$ chosen suitably. For this map, c,

$$\sum_S (-1)^{|S \cap T|} c_S$$

and

$$\sum_S (-1)^{|S \cap T^c|} c_S$$

are equivalent. To obtain the required inequalities as given in the theorem, it is then enough choose δ such that (3.1.5) holds for $T = \phi, \{i\}$ (for $i = 1, 2, 3, 4$) and $\{1, 2\}, \{1, 3\}, \{1, 4\}$.

Thus, we have a small set of simple verifiable conditions for spin correlation matrices of order $n \leq 4$. One can construct simple examples to see that the above result does not extend to say $n \geq 5$. Here's an example for $n = 5$.

Example 3. *We have $n = 5$ and $c_{ii} = 1$ for all $1 \leq i \leq 5$. Let*

$$c_{ij} = \begin{cases} \theta & \text{if } \ i = 1 \\ \rho & \text{otherwise} \end{cases}$$

Then, the Bell's inequalities reduce to

$$-\frac{1}{3} \leq \rho \leq 1$$

$$-1 + 2\theta + \rho \geq 0$$

$$1 - 2\theta + \rho \geq 0$$

For, $C = ((c_{ij}))$ to be a correlation matrix it has to be positive semi-definite. The conditions for positive semi-definiteness come out to be

$$\theta^2 \leq \frac{1}{4}(1 + 3\rho)$$

For $\theta = \frac{1}{4}$ and $\rho = -\frac{7}{24}$, Bell's inequalities are satisfied but not that of positive semi-definiteness. Another interesting example is when $C \notin \mathrm{Cov}_n$ but satisfies the above inequalities. This happens for $\theta = \frac{1}{4}$ and $\rho = -\frac{5}{24}$. Thus, for $n = 5$, the conditions of bell's inequalities are not sufficient for C to be a spin correlation matrix.

Before going into details of obtaining similar results for large n, we divert our attention to a related problem of vertex enumeration. The V-representation of spin correlation is knowns and is rather simple understand.

3.1.2 Complete Characterization in terms of extremals

In Parthasarathy's paper, he asks the question of extremals of spin variables. The complete characterisation of extremals of spin correlations was given by J. C. Gupta in 1999 [16]. Let us establish some notation before stating the main theorem.

Define coordinate projections on Ω_n as $\xi_i(\sigma) = \sigma_i, 1 \leq i \leq n$. For $T \subset \{1, 2, \ldots, n\}$, denote by σ^T the configuration σ such that $\sigma_i = -1$ for all $i \in T$ and $\sigma_j = 1$ for all $j \in T^c$. We introduce probability P^T as follows:

$$P^T(\{\sigma^T\}) = P^T(\{\sigma^{T^c}\}) = \frac{1}{2}$$

The, under P^T, $\xi_1, \xi_2, \ldots, \xi_n$ are spin variable with correlation matrix

$\Sigma^T = ((c_{ij}^T))$ where $c_{ii}^T = 1$ for all i and $c_{ij}^T = (-1)^{|T \cap \{i,j\}|}$ for $i \neq j$.

Note that $P^T = P^{T^c}$ and the set $\{\Sigma^T : T \in \mathcal{T}\}$, where $\mathcal{T} = \{T \subset \{1, 2, \ldots, n\} : 1 \in T\}$, consists of 2^{n-1} distinct spin correlation matrices of order n. These matrices are in fact the extremals of the

convex hull of realizable spin correlation matrices.

Theorem 3.1.5. *(J. C. Gupta, 1999): The class of realizable correlation matrices of n spin variables is given by*

$$\mathrm{Cov}_n = ConvexHull\{\Sigma^T : T \in \mathcal{T}\}$$

where Σ^T and $\mathcal{T}$ are defined as follows:

$$\mathcal{T} = \{T \subset \{1, 2, \ldots, n\} : 1 \in T\}$$

and

$$\Sigma^T = ((c_{ij}^T))$$

where $c_{ii}^T = 1$ for all i and $c_{ij}^T = (-1)^{|T \cap \{i,j\}|}$ for $i \neq j$

Proof. Sufficiency: Clearly the matrix $\sum \lambda_T \Sigma^T; \lambda_T \geq 0, \sum \lambda_T = 1$ is a correlation matrix of $\xi_1, \xi_2, \ldots \xi_n$ under the probability $P = \sum \lambda_T P^T$ on Ω_n

Necessity: Let Δ be the correlation matrix of n spins $\eta_1, \eta_2, \ldots, \eta_n$ defined on a probability space $(\Omega, \mathcal{F}, Q)$. On Ω_n define P as follows:

$$P(\{\sigma^T\}) = P(\{\sigma^{T'}\}) = \frac{1}{2}Q\{\eta_i = -1 \ \forall \ i \in T, \eta_j = 1 \ \forall j \ \notin T\}$$
$$+\frac{1}{2}Q\{\eta_i = 1 \ \forall \ i \in T, \eta_j = -1 \ \forall j \ \notin T\}; \text{ where } T \in \mathcal{T}$$

Under P, $\xi_1, \xi_2, \ldots, \xi_n$ are spin variables with the correlation matrix Δ. Clearly $P = \sum_T \lambda_T P^T$ with $\lambda_T = P(\{\sigma^T\}) + P(\{\sigma^{T'}\})$ so that $\Delta = \sum \lambda_T \Sigma^T \in \mathrm{Cov}_n$

□

The set $\{\Sigma^T : T \in \mathcal{T}\}$ is in fact the set of extremals. Indeed, there are 2^n vectors of the form $\xi = (\xi_1, \xi_2, \ldots, \xi_n)$ where $\xi = \pm 1$. These form the vertices of an $n-$dimensional cube. The vectors $a^T = (c_{11}^T, c_{12}^T, \ldots, c_{1,n}^T, c_{23}^T, \ldots, c_{2,n}^T, \ldots\ldots c_{n-1,n}^T)$ are subset of the set of 2^n ξ's. Clearly $conv(\{\xi\}) \subset conv(\{a^T\})$. Since, ξ's form the vertices of the cube, the a^Ts must form the vertices of the convex hull $conv(\{a^T\})$. This implies that the matrices σ^Ts are the vertices of Cov_n.

Now we have a complete description of Cov_n in terms of extremals, for all n. However, given a matrix C, it is still very difficult to determine whether C is inside Cov_n or not. For this purpose, a V-representation of Cov_n is desirable. We already have a V-representation of Cov_n for $n \leq 4$. Let us look at the V-representation and the H-representation for spin correlation matrices of order $n = 3$.

Example 4. *Take n = 3. Then,*

$$\mathcal{T} = \{\{1\}, \{1, 2\} \{1, 3\} \{1, 2, 3\}\}$$

the corresponding correlation matrices that are the extremals of the space of spin correlation matrices of order n are

$$M_1 = \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{pmatrix}, \qquad M_2 = \begin{pmatrix} 1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix},$$
$$M_3 = \begin{pmatrix} 1 & -1 & 1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \end{pmatrix}, \qquad M_4 = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

The corresponding Bell's inequalities are

$$\begin{aligned} 1 + c_{12} + c_{23} + c_{13} &\geq 0 \\ 1 - c_{12} - c_{23} + c_{13} &\geq 0 \\ 1 - c_{12} + c_{23} - c_{13} &\geq 0 \\ 1 + c_{12} - c_{23} - c_{13} &\geq 0 \end{aligned}$$

Take a matrix M in Cov_4. Then, we can write $M = \sum_{i=1}^{4} \alpha_i M_i$ such that $\sum_{i=1}^{4} \alpha_i = 1$ and $0 \leq \alpha_i \leq 1$ for all $i = 1, \ldots, 4$. That is,

$$M = \begin{pmatrix} 1 & -\alpha_1 + \alpha_2 - \alpha_3 + \alpha_4 & -\alpha_1 - \alpha_2 + \alpha_3 + \alpha_4 \\ -\alpha_1 + \alpha_2 - \alpha_3 + \alpha_4 & 1 & \alpha_1 - \alpha_2 - \alpha_3 + \alpha_4 \\ -\alpha_1 - \alpha_2 + \alpha_3 + \alpha_4 & \alpha_1 - \alpha_2 - \alpha_3 + \alpha_4 & 1 \end{pmatrix}$$

So, we have

$$\begin{aligned} -\alpha_1 + \alpha_2 - \alpha_3 + \alpha_4 &= c_{12} \\ -\alpha_1 - \alpha_2 + \alpha_3 + \alpha_4 &= c_{31} \\ \alpha_1 - \alpha_2 - \alpha_3 + \alpha_4 &= c_{23} \\ \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 &= 1 \end{aligned}$$

It is interesting to see that, solving these for α_i and imposing the condition $\alpha_i \geq 0$ for all $i = 1, \ldots, 4$ gives precisely the Bell's inequality.

In the following discussion in this chapter we will try to obtain a general description of inequalities (in other words the H-representation) for any n and some explicitly verifiable inequalities for small n.

3.2 Maximum Entropy Method

Consider the function $h(x) = -x \log x$ where $x \in \mathbb{R}, x > 0$. Notice that $\lim_{x\to 0} h(x) = 0$. So, we can extend the domain of h to all of $x \geq 0$. Now, for a discrete probability distribution P on the countable set $\{x_1, x_2, ...\}$, with $P_i = P(x_i)$, the entropy of P is defined as

$$S(P) = -\sum_i P_i \log P_i$$

In case when the state space is not discrete, for a probability density function $P(x)$ on $\mathbb{R}$, the entropy can be defined as

$$S(P) = -\int P(x) \log P(x) dx$$

This definition of entropy was introduced by Shannon and resembles the thermodynamic notion of entropy. This form of entropy with base 2 logarithm (to express it in bits) is used in Information Theory. Physically, entropy measures how disordered a system is. Systems are expected to evolve into states with higher entropy as they approach equilibrium. In probabilistic context, $S(P)$ is viewed as a measure of the information carried by P, with higher entropy corresponding to less information and more uncertainty.

The Principle of Maximum Entropy is based on the premise that when estimating the probability distribution, one should select that distribution which leaves the largest remaining uncertainty (i.e., the maximum entropy) consistent with the given constraints. That way we can ensure that we have not introduced any additional assumptions or biases into our calculations.
So, if we are seeking a probability density function subject to certain constraints (e.g., a given mean or variance or higher moments), it is desirable to use the density satisfying those constraints that has entropy as large as possible. Any probability density function satisfying the constraints that has smaller entropy will contain more information (less uncertainty), and thus says something stronger than what we are assuming.

Example 5. *Consider a finite set $A = \{x_1, x_2, \ldots, x_n\}$. Let us see what different probability distributions mean in terms of entropy. Suppose, we have probability on A denoted by P such that $P(x_1) = 1$ and $P(x_i) = 0$ for all $1 < i \leq n$. Then, the entropy $S(P) = -1log1 = 0$. Thus, we see that the measure of disorder, the entropy is zero when P is such that there is only one possible outcome and there is no uncertainty. On the other hand, when we consider the uniform density, that is, $P(x_i) = 1/n$ for all i, the entropy comes out to be $S(P) = \log n$. As we will see next, this is the maximum entropy over all possible distributions. Since the uniform distribution gives us minimum information (or highest uncertainty of outcome), the entropy is maximum is this case.*

Theorem 3.2.1. *For a probability density function P on a finite set $\{x_1, x_2, \ldots, x_n\}$,*

$$S(P) \leq \log n$$

with equality if and only if P is uniform, i.e. $P(x_i) = 1/n$ for all i.

Proof. A probability density function on $\{x_1, \ldots, x_n\}$ is a set of nonnegative real numbers $P = (p_1, \ldots, p_n)$ that add up to 1. Entropy is a continuous function of the n-tuples $(p_1, \ldots, p_n)$, and

these points lie in a compact subset of $\mathbb{R}^n$, so there is an n-tuple where entropy is maximized. We want to show this occurs at $(1/n, ..., 1/n)$ and nowhere else.

Suppose that the p_j's are not all equal, say $p_1 < p_2$. We will show that there exists a new probability density with higher entropy. It then follows, since entropy is maximized at some n-tuple, that entropy is uniquely maximized at the n-tuple with $p_i = 1/n$ for all i.

Since $p_1 < p_2$, for $\varepsilon > 0$ small, we have $p_1 + \varepsilon < p_2 - \varepsilon$. Denote by Q, the $n-$tuple $(p_1 + \varepsilon, p_2 - \varepsilon, p_3, \ldots, p_n)$. Then the difference in entropies is given by

$$\begin{aligned} S(Q) - S(P) = &-p_1 \log\left(\frac{p_1 + \varepsilon}{p_1}\right) - \varepsilon \log(p_1 + \varepsilon) \\ &-p_2 \log\left(\frac{p_2 - \varepsilon}{p_2}\right) + \varepsilon \log(p_2 - \varepsilon) \end{aligned}$$

Or,

$$\begin{aligned} S(Q) - S(P) = &-p_1 \log\left(1 + \frac{\varepsilon}{p_1}\right) - \varepsilon \left(\log p_1 + \log\left(1 + \frac{\varepsilon}{p_1}\right)\right) \\ &-p_2 \log\left(1 - \frac{\varepsilon}{p_2}\right) + \varepsilon \left(\log p_2 + \log\left(1 - \frac{\varepsilon}{p_2}\right)\right) \end{aligned}$$

Now, since $\log(1 + x) = x + O(x^2)$ for small x, we get

$$\begin{aligned} S(Q) - S(P) &= -\varepsilon - \varepsilon \log p_1 + \varepsilon \log p_2 + O(\varepsilon^2) \\ &= \varepsilon \log(p_2/p_1) + O(\varepsilon^2) \end{aligned}$$

which is positive since $p_1 < p_2$. This implies $S(Q) - S(P) > 0$ for ε sufficiently small. □

In continuous case there are similar results which we state here without proofs.

Theorem 3.2.2. *For a probability density function p on $\mathbb{R}$ with variance σ^2,*

$$S(p) \leq \frac{1}{2}(1 + \log(2\pi\sigma^2))$$

with equality if and only if p is Gaussian with variance σ^2.

Theorem 3.2.3. *For a probability density function p on $(0, \infty)$ with mean μ,*

$$S(p) \leq 1 + \log \mu$$

with equality if and only if p is exponential with mean μ.

Note that there can be cases where a maximum entropy distribution may not exist. If we extend the above theorem to consider the set of probability density functions on $\mathbb{R}$ with fixed mean μ, we will find that no maximum entropy distribution exists in this case. The one-dimensional Gaussians with mean μ and increasing variance have no maximum entropy.

Before proceeding to uniqueness question, we will look at some interesting properties of the entropy function that arise from special properties of the function $h(x) = -x \log x$.

Lemma 3.2.1. *For continuous probability density functions p and q on $\mathbb{R}$, with $p \geq 0$ and $q > 0$,*

$$-\int_{\mathbb{R}} p \log p dx \leq -\int_{\mathbb{R}} p \log q dx$$

if both integrals exist. Moreover, there is equality if and only if $p(x) = q(x)$ almost everywhere.

For discrete probability density functions p and q on a set $\{x_1, x_2, \ldots.\}$, with $p(x_i) \geq 0$ and $q(x_i) > 0$ for all i,

$$-\sum_{i \geq 1} p(x_i) \log p(x_i) \leq -\sum_{i \geq 1} p(x_i) \log q(x_i)$$

if both sums converge. Moreover, there is equality if and only if $p(x_i) = q(x_i)$ for all i.

Proof. We only give the proof of the continuous case here. The proof for the discrete case is identical. First of all, notice that for $x > 0$ and $y \geq 0$

$$y - y \log y \leq x - y \log x$$

Indeed, the above holds for $y = 0$. For $y > 0$, it is east to see that $\log(x/y) \leq x/y - 1$ golds with equality if and only if $x = y$. Then, for any $x \in \mathbb{R}$ we get,

$$p(x) - p(x) \log p(x) \leq q(x) - p(x) \log q(x)$$

Integrating this gives

$$-\int_{\mathbb{R}} p \log p dx \leq -\int_{\mathbb{R}} p \log q dx$$

If there is equality, then

$$\int_{\mathbb{R}} [q(x) - p(x) \log q(x) - p(x) + p(x) \log p(x)] dx = 0$$

Note that $q(x) - p(x) \log q(x) - p(x) + p(x) \log p(x)$ is a non-negative continuous function whose integral over $\mathbb{R}$ is zero. This means $q(x) - p(x) \log q(x) - p(x) + p(x) \log p(x) = 0$ almost everywhere. Then from continuity and from the above discussion it follows that $p(x) = q(x)$ almost everywhere. □

Remark 3.2.1. Notice that theorem 3.2.1 follows easily from the above result. By letting $q_i = 1/n$ for all i,

$$-\sum_{i=1}^{n} p_i \log q_i = \sum_{i=1}^{n} p_i \log n = \log n,$$

which is the entropy of q. Therefore we have $S(p) \leq S(q)$, with equality if and only if p is uniform.

We will now prove a uniqueness result for probability measure with maximum entropy. To make the discussion fairly broad, we will work in the general context of entropy on measure spaces. Let $(\mathcal{E}, \nu)$ be a measure space. A probability density function p on $(\mathcal{E}, \nu)$ is a ν-measurable function

from $\mathcal{E}$ to $[0,\infty)$ such that $pd\nu$ is a probability measure on $\mathcal{E}$. Define the entropy of p to be

$$S(p) = -\int_{\mathcal{E}} p\log p d\nu$$

assuming this converges. That is, we assume $p\log p \in L^1(\mathcal{E},\nu)$. (Note the entropy of p depends on the choice of ν). For any probability measure μ on $\mathcal{E}$ that is absolutely continuous with respect to ν, we can define the entropy of μ with respect to ν as $-\int_{\mathcal{E}}\log(d\mu/d\nu)d\mu$ where $d\mu/d\nu$ is the Radon-Nikodym derivative.

Let Π be any set of probability density functions p on $(\mathcal{E},\nu)$ that is closed under convex-linear combinations and let Π' be the subset of Π consisting of those $p\in\Pi$ with finite entropy. We will see that Π' is closed under convex-linear combinations.

We now state two important lemmas that are crucial in arriving at the the uniqueness result.

Lemma 3.2.2. *The probability density functions on $(\mathcal{E},\nu)$ having finite entropy are closed under convex-linear combinations if $S(p_1)$ and $S(p_2)$ are finite, so is $S((1-\varepsilon)p_1+\varepsilon p_2)$ for any $\varepsilon\in[0,1]$.*

Proof. We may take $0<\varepsilon<1$. Let $f(t)=-t\log t$ for $t\geq 0$, so $S(p)=\int_{\mathcal{E}} f(p(x))d\nu(x)$. From the concavity of the graph of s,

$$f((1-\varepsilon)t_1+\varepsilon t_2)\geq(1-\varepsilon)f(t_1)+\varepsilon f(t_2)$$

when $t_1,t_2\geq 0$. Therefore,

$$f((1-\varepsilon)p_1(x)+\varepsilon p_2(x))\geq(1-\varepsilon)f(p_1(x))+\varepsilon f(p_2(x))$$

For an upper bound on $f((1-\varepsilon)t_1+\varepsilon t_2)$, we note that $f(t_1+t_2)\leq f(t_1)+f(t_2)$ for all $t_1,t_2\geq 0$. This is clear if either t_1 or t_2 is 0. When t_1 and t_2 are both positive,

$$\begin{aligned} f(t_1+t_2) &= -(t_1+t_2)\log(t_1+t_2)\\ &= -t_1\log(t_1+t_2)-t_2\log(t_1+t_2)\\ &\leq -t_1\log(t_1)-t_2\log(t_2)\\ &= f(t_1)+f(t_2)\end{aligned}$$

Therefore,

$$(1-\varepsilon)f(p_1(x))+\varepsilon f(p_2(x))\leq f((1-\varepsilon)p_1(x)+\varepsilon p_2(x))\leq f((1-\varepsilon)p_1(x))+f(\varepsilon p_2(x)).$$

Integrate this over $\mathcal{E}$. Since $\int_{\mathcal{E}} f(\delta p(x))dx=-\delta\log\delta+\delta S(p)$ for $\delta\geq 0$ and p a probability distribution on $\mathcal{E}$, we see $(1-\varepsilon)p_1+\varepsilon p_2$ has finite entropy:

$$(1-\varepsilon)S(p_1)+\varepsilon S(p_2)\leq S((1-\varepsilon)p_1+\varepsilon p_2)\leq -(1-\varepsilon)\log(1-\varepsilon)+(1-\varepsilon)S(p_1)-\varepsilon\log\varepsilon+\varepsilon S(p_2).$$

□

Lemma 3.2.3. *If there are p_1 and p_2 in Π' such that on the subset $A\subset\mathcal{E}$, $p_1=0$ and $p_2>0$, then*

$$S((1-\varepsilon)p_1 + \varepsilon p_2) > S(p_1)$$

for any positive ε, sufficiently small.

Proof. Let $B = \mathcal{E} \setminus A$, so $S(p_1) = -\int_A p_1 \log p_1 d\nu$. Since p_1 and p_2 are in Π', $(1-\varepsilon)p_1 + \varepsilon p_2 \in \Pi'$ for any $\varepsilon \in [0,1]$.

As in the proof of Lemma 3.2.2, let $f(t) = -t \log t$ for $t \geq 0$. Since $p_1 = 0$ on A,

$$S(p_1) = \int_{\mathcal{E}} f(p_1) d\nu = \int_B f(p_1) d\nu$$

Then,

$$\begin{aligned}
S((1-\varepsilon)p_1 + \varepsilon p_2) &= \int_A f((1-\varepsilon)p_1 + \varepsilon p_2) d\nu + \int_B f((1-\varepsilon)p_1 + \varepsilon p_2) d\nu \\
&= \int_A f(\varepsilon p_2) d\nu + \int_B f((1-\varepsilon)p_1 + \varepsilon p_2) d\nu \\
&\geq \int_A f(\varepsilon p_2) d\nu + \int_B ((1-\varepsilon) f(p_1) + \varepsilon f(p_2)) d\nu \\
&= \varepsilon S(p_2) - (\varepsilon \log \varepsilon) \int_A p_2 d\nu + (1-\varepsilon) S(p_1) \\
&= S(p_1) + \varepsilon(-(\log \varepsilon) \int_A p_2 d\nu + S(p_2) - S(p_1)).
\end{aligned}$$

Since $\nu(A) > 0$ and $p_2 > 0$ on A, $\int_A p_2 d\nu$. Therefore the expression inside the parentheses is positive when ε is close enough to 0, no matter the size of $S(p_2) - S(p_1)$. Thus, the overall entropy is greater than $S(p_1)$ for small ε. □

Theorem 3.2.4. *If Π' contains a probability density function q with maximum entropy, then every $p \in \Pi'$ vanishes almost everywhere q vanishes.*

Proof. If the statement is false, then there is some $p \in \Pi'$ and some $A \subset \mathcal{E}$ with $\nu(A) > 0$ such that, on A, $q = 0$ and $p > 0$. However, for sufficiently small $\varepsilon > 0$, the probability density function $(1-\varepsilon)q + \varepsilon p$ lies in Π' and has greater entropy that q by lemma 3.2.3. This is a contradiction. □

Theorem 3.2.5. *If q_1 and q_2 have maximum entropy in Π', then $q_1 = q_2$ almost everywhere.*

Proof. By theorem 3.2.4, we can change q_1 and q_2 on the set of measure 0 in order to assume they have the same zero set, say Z. Let $Y = \mathcal{E} \setminus Z$. Then, q_1 and q_2 are positive probability density functions on Y.

Let $q = \frac{1}{2}(q_1 + q_2)$. Then $q > 0$ on Y. By lemma 3.2.2, $q \in \Pi'$. By lemma 3.2.1,

$$S(q_1) = -\int_Y q_1 \log q_1 d\nu \leq \int_Y q_1 \log q d\nu$$

and

$$S(q_2) = -\int_Y q_2 \log q_2 d\nu \leq \int_Y q_2 \log q d\nu$$

$$\begin{aligned} S(q) &= -\int_S q \log q d\nu \\ &= -\int_Y q \log q d\nu \\ &= -\frac{1}{2}\int_Y q_1 \log q - \frac{1}{2}\int_Y q_2 \log q \\ &\geq \frac{1}{2}(S(q_1) + S(q_2)) \\ &= S(q_1) \end{aligned}$$

maximality implies $S(q) = S(q_1) = S(q_2)$. This implies

$$\begin{aligned} S(q_1) &= -\int_Y q_1 \log q_1 d\nu = \int_Y q_1 \log q d\nu \\ S(q_2) &= -\int_Y q_2 \log q_2 d\nu = \int_Y q_2 \log q d\nu \end{aligned}$$

Then, by lemma 3.2.1, $q_1 = q = q_2$ almost everywhere on Y. So, $q_1 = q_2$ almost everywhere on S.

□

Remark 3.2.2. We have stated earlier (Theorem 3.2.2) that for a probability density function p on $\mathbb{R}$ with variance σ^2 there are infinitely many maximum entropy distributions, namely, all Gaussians on $\mathbb{R}$ with a fixed variance (σ^2) have the same entropy. This does not a contradict Theorem 3.2.5, since the property of having a fixed variance is not closed under convex-linear combinations.

Since, we are going to look at covariance realization problems, we are going to have constraints in the form of fixed covariances. We will look at a maximum entropy solution (using Lagrange multipliers) for spin systems. For the sake of completion, we state a corresponding result (without proof) in case of multi-dimensional processes.

Theorem 3.2.6. *For a continuous probability density function p on $\mathbb{R}^n$ with fixed covariances c_{ij},*

$$S(p) \leq \frac{1}{2}(n + \log((2\pi)^n \det \Sigma))$$

where $\Sigma = ((c_{ij}))$ is the covariance matrix for p. There is equality if and only if p is an n-dimensional Gaussian density with covariances c_{ij}.

3.2.1 Lagrange Multiplier Method

As we have seen, the entropy has its maximum value when all probabilities are equal (we again assume the number of possible states is finite), and the resulting value for entropy is the logarithm of the number of states. If we have no additional information about the system, then such a result seems reasonable. The moments or the covariances provide us this extra information or constraint. To find a distribution that maximizes the entropy as well as satisfies the constraints on can use techniques from calculus of variations. The Lagrange Multipliers Method is often used in this context. One of the most common problems in calculus is that of finding extrema of a function. The problem is that it is often difficult to find a closed form when one wishes to maximize or minimize a function subject to fixed constraints. The method of Lagrange multipliers is a powerful tool for solving this kind of problems without the need to explicitly solve the conditions.The technique is named after the famous mathematician, Joseph-Louis Lagrange.

We consider a very general optimization problem given by

$$\text{minimize } f_0(x) \text{ on } M, \text{where } M \text{ is the set determined by the constraints:}$$
$$f_i(x) \leq 0 \; i = 1, \ldots, m$$
$$h_i(x) = 0 \; i = 1, \ldots, p$$

where, $f_0 : Y \longrightarrow \mathbb{R}$ for non-empty set Y and $M \subset Y$, M is non-empty. We assume that the domain $D = (\cap_{i=1}^{m} \text{ dom } f_i) \cap (\cap_{i=1}^{p} \text{ dom } h_i)$ is non-empty. In order to solve this constrained optimization problem one can use the Lagrange Multiplier Method.

Definition 3.2.1. The map $\Lambda : Y \longrightarrow \mathbb{R}$ is called a Lagrange Functional for the optimization problem if it is finite and constant over M.

Lemma 3.2.4. *(Lagrange Lemma) Let $\Lambda : Y \longrightarrow \mathbb{R}$ be a Lagrange functional and let $y_0 \in M$ minimizes $\mathcal{L} = \mathcal{H} + \Lambda$ over Y. Then, y_0 minimizes $\mathcal{H}$ over M.*

Notice that the above result does not require any algebraic nor topological structure on Y and the hypotheses on Λ are also minimal. The proof is rather simple and follows from the definition of Lagrange functional.

Proof. For any $y \in M$, we have $f_0(y_0) + \Lambda(y_0) \leq f_0(y) + \Lambda(y) = f_0(y) + \Lambda(y_0)$. Hence, $f_0(y_0) \leq f_0(y)$. □

The Lagrange dual function

Consider the optimization problem $\mathfrak{P}$ [4].

$$\begin{aligned} \text{minimize} \quad & f_0(x) \\ \text{subject to} \quad & f_i(x) \leq 0 \; i = 1, \ldots, m \\ & h_i(x) = 0 \; i = 1, \ldots, p \end{aligned}$$

such that the domain D defined as above is non-empty. We denote the optimal value (if it exists) by p^*. The Lagrangian $\mathcal{L} : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^p \longrightarrow \mathbb{R}$, as defined above, is given by

$$\mathcal{L}(x, \lambda, \nu) = f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) + \sum_{i=1}^{p} \nu_i h_i(x)$$

where λ_i and ν_i are Lagrange multipliers.

Then, the (Lagrange) dual function is defined as a function $g : \mathbb{R}^{m+p} \longrightarrow \mathbb{R}$ which is the minimum of $\mathcal{L}$ over x. That is,

$$g(\lambda, \nu) = \inf_{x \in D} \mathcal{L}(x, \lambda, \nu)$$

When the Lagrangian is unbounded below in x, the dual function takes on the value $-\infty$.

The dual function yields lower bounds on the optimal value p^*. For any $\lambda \geq 0$ and ν we have

$$g(\lambda, \nu) \leq p^*$$

Indeed, if x^* is any feasible point of the given optimization problem, then we have that $f_i(x^*) \leq 0$ and $h_i(x^*) = 0$ and hence

$$\mathcal{L}(x^*, \lambda, \nu) = f_0(x^*) + \sum_{i=1}^{m} \lambda_i f_i(x^*) + \sum_{i=1}^{p} \nu_i h_i(x^*) \leq f_0(x^*)$$

Since, $\lambda_i \geq 0$, we have

$$g(\lambda, \nu) = \inf_{x \in D} \mathcal{L}(x, \lambda, \nu) \leq \mathcal{L}(x^*, \lambda, \nu) \leq f_0(x^*)$$

Since the above holds for every feasible point, it implies that

$$g(\lambda, \nu) \leq p^*$$

.

The Lagrange Dual Problem

For each pair (λ, ν) with $\lambda \geq 0$, the Lagrange dual function gives us a lower bound on the optimal value p^* of the optimization problem $\mathfrak{P}$. Thus we have a lower bound that depends on some parameters (λ, ν). A natural question is: what is the best lower bound that can be obtained from the Lagrange dual function? This leads to the optimization problem

$$\begin{array}{ll} \text{maximize} & g(\lambda, \nu) \\ \text{subject to} & \lambda \geq 0 \end{array}$$

This problem is called the Lagrange dual problem associated with the problem $\mathfrak{P}$. In this context the original problem is sometimes called the primal problem.

Let us consider a more concrete example of this. Consider the following problem

$$\begin{aligned} \text{minimize} \quad & c^T x \\ \text{subject to} \quad & Ax = b \\ & x \geq 0 \end{aligned}$$

The Lagrangian function is given by

$$\begin{aligned} \mathcal{L}(x, \lambda, \nu) &= c^T x - \sum_{i=1}^{m} \lambda_i x_i + \nu^T (Ax - b) \\ &= -b^T \nu + (c + A^T \nu - \lambda)^T x \end{aligned}$$

The dual function is

$$\begin{aligned} g(\lambda, \nu) &= \inf_x \mathcal{L}(x, \lambda, \nu) \\ &= -b^T \nu + \inf_x (c + A^T \nu - \lambda)^T x \end{aligned}$$

which is easily determined analytically, since a linear function is bounded below only when it is identically zero. Thus, $g(\lambda, \nu) = -\infty$ except when $c + A^T \nu - \lambda = 0$, in which case it is $-b^T \nu$

$$g(\lambda, \nu) = \begin{cases} -b^T \nu & \text{if } A^T \nu - \lambda + c = 0 \\ -\infty & \text{otherwise} \end{cases}$$

Note that the dual function g is finite only on a proper affine subset of (λ, ν). Strictly speaking, the Lagrange dual problem is to maximize this dual function g, that is,

$$\begin{aligned} \text{maximize} \quad & g(\lambda, \nu) = \begin{cases} -b^T \nu & \text{if } A^T \nu - \lambda + c = 0 \\ -\infty & \text{otherwise} \end{cases} \\ \text{subject to} \quad & \lambda \geq 0. \end{aligned}$$

Here g is finite only when $A^T \nu - \lambda + c = 0$. We can form an equivalent problem by making these equality constraints explicit:

$$\begin{aligned} \text{maximize} \quad & -b^T \nu \\ \text{subject to} \quad & A^T \nu - \lambda + c = 0 \\ & \lambda \geq 0 \end{aligned}$$

This problem, in turn, can be expressed as

$$\begin{aligned} \text{maximize} \quad & -b^T \nu \\ \text{subject to} \quad & A^T \nu + c = 0 \end{aligned}$$

We will now use the Lagrange multiplier method to get a maximum entropy solution for spin variables.

3.2.2 Maximum Entropy Measure for Spins

We employ the same technique of Lagrange multipliers to solve the optimization problem of maximizing the entropy under given constraints of fixed spin correlations. Thus, given

$$c_{hk} = \sum_{\sigma} \sigma_h \sigma_k \mathcal{P}(\sigma)$$

we want to find a density function for the spin random variables such that it maximizes the entropy. Note that the entropy is defined as -

$$\mathcal{S}(\mathcal{P}(\sigma)) = -\sum_{\sigma} \mathcal{P}(\sigma) \log \mathcal{P}(\sigma)$$

To do so we use the Lagrange method. In addition to the above constraints we would also want -

$$\sum_{\sigma} \mathcal{P}(\sigma) = 1$$

Thus we have the following constraints:

$$\sum_{\sigma} \sigma_h \sigma_k \mathcal{P}(\sigma) = c_{hk}. \tag{3.2.1}$$

$$\sum_{\sigma} \mathcal{P}(\sigma) = 1 \tag{3.2.2}$$

We want to maximize $\mathcal{S}$. Consider the *Lagrangian function* -

$$\mathcal{L}(\mathcal{P}(\sigma) = \Lambda(\mathcal{P}(\sigma)) + \mathcal{S}(\mathcal{P}(\sigma))$$

where $\Lambda(\mathcal{P}(\sigma))$ is a *Langrage functional* defined as -

$$\Lambda(\mathcal{P}(\sigma)) = \sum_{h,k} \lambda_{hk} \left(c_{hk} - \sum_{\sigma} \sigma_h \sigma_k \mathcal{P}(\sigma) \right) + \mu \left(\sum_{\sigma} \mathcal{P}(\sigma) - 1 \right)$$

Notice that $\Lambda(\mathcal{P}(\sigma))$ is constant (in fact, it is zero) on the space -

$$M = \left\{ \mathcal{P}(\sigma) | \mathcal{P}(\sigma) \geq 0, \sum_{\sigma} \mathcal{P}(\sigma) = 1, \sum_{\sigma} \sigma_h \sigma_k \mathcal{P}(\sigma) = c_{hk} \right\}$$

where $\lambda_{hk}, \mu \in \mathbb{R}$ are the *Lagrange multipliers*. Now,

$$\mathcal{L}(\mathcal{P}(\sigma)) = \sum_{h,k} \lambda_{hk} \left(c_{hk} - \sum_{\sigma} \sigma_h \sigma_k \mathcal{P}(\sigma) \right) + \mu \left(\sum_{\sigma} \mathcal{P}(\sigma) - 1 \right) - \sum_{\sigma} \mathcal{P}(\sigma) \log \mathcal{P}(\sigma)$$

Leaving out the constants what remains as a functions of $\mathcal{P}$ is -

$$\begin{aligned} \mathcal{I}(\mathcal{P}) &= -\sum_{\sigma} \mathcal{P}(\sigma) \log \mathcal{P}(\sigma) - \sum_{h,k} \lambda_{hk} \sum_{\sigma} \sigma_h \sigma_k \mathcal{P}(\sigma) + \mu \sum_{\sigma} \mathcal{P}(\sigma) \\ &= \sum_{\sigma} \mathcal{P}(\sigma) \left[-\log \mathcal{P}(\sigma) - \sum_{h,k} \lambda_{hk} \sigma_h \sigma_k + \mu \right] \end{aligned}$$

$\mathcal{I}(\mathcal{P})$ is a function of 2^n variables (for each σ). We consider partial derivative of $\mathcal{I}$. We denote by $\partial_P \mathcal{I}(P(\sigma))$ the partial derivative with respect to $\mathcal{P}(\sigma)$. We have,

$$\partial_P \mathcal{I}(\mathcal{P}(\sigma)) = -\log \mathcal{P}(\sigma) - \sum_{h,k} \lambda_{hk} \sigma_h \sigma_k + \mu - 1$$

Thus, the gradient of $\mathcal{I}(\mathcal{P})$ is clearly zero at the point,

$$\mathcal{P}^*(\sigma) = \frac{1}{Z} \exp \left\{ -\sum_{h,k} \lambda_{hk} \sigma_h \sigma_k \right\}$$

where $Z = \exp\{\mu - 1\}$. Note that any probability of this form is such that $\mathcal{P}^*(\sigma) = \mathcal{P}^*(-\sigma)$. In particular, this implies that each spin has mean zero with respect to $\mathcal{P}^*$. Let us now look at the dual problem.

Dual Problem

$$\begin{aligned} \Lambda(\mathcal{P}(\sigma)) &= \mu \left(\sum_{\sigma} \mathcal{P}(\sigma) - 1 \right) + \sum_{h,k} \lambda_{hk} \left(c_{hk} - \sum_{\sigma} \sigma_h \sigma_k \mathcal{P}(\sigma) \right) \\ &= \sum_{h,k} \lambda_{hk} c_{hk} - \sum_{\sigma} \sum_{h,k} \lambda_{hk} \sigma_h \sigma_k \mathcal{P}(\sigma) \end{aligned} \tag{3.2.3}$$

(Since $\sum_{\sigma} \mathcal{P}(\sigma) = 1$). Also,

$$\begin{aligned}
\mathcal{S}(\mathcal{P}(\sigma)) &= -\sum_{\sigma}\left[\left(\frac{1}{Z}\exp\left\{-\sum_{h,k}\lambda_{hk}\sigma_h\sigma_k\right\}\right)\log\left(\frac{1}{Z}\exp\left\{-\sum_{h,k}\lambda_{hk}\sigma_h\sigma_k\right\}\right)\right] \\
&= \sum_{\sigma}\left[\left(\frac{1}{Z}\exp\left\{-\sum_{h,k}\lambda_{hk}\sigma_h\sigma_k\right\}\right)\left(\left\{\sum_{h,k}\lambda_{hk}\sigma_h\sigma_k\right\}\right)\right] \\
&\quad + \log Z\left[\sum_{\sigma}\left(\frac{1}{Z}\exp\left\{-\sum_{h,k}\lambda_{hk}\sigma_h\sigma_k\right\}\right)\right] \\
&= \log Z + \left\{\sum_{h,k}\lambda_{hk}\sigma_h\sigma_k\right\}\left[\sum_{\sigma}\frac{1}{Z}\exp\left\{-\sum_{h,k}\lambda_{hk}\sigma_h\sigma_k\right\}\right] \\
&= \log Z + \sum_{\sigma}\sum_{h,k}\lambda_{hk}\sigma_h\sigma_k\mathcal{P}(\sigma) \qquad (3.2.4)
\end{aligned}$$

From (3.2.3) and (3.2.4) we get -

$$\mathcal{L}(\mathcal{P}(\sigma)) = \Lambda(\mathcal{P}(\sigma)) + \mathcal{S}(\mathcal{P}(\sigma)) = \log Z + \sum_{h,k}\lambda_{hk}c_{hk}$$

Writing this as a function of $\lambda'_{hk}s$ we get -

$$\mathcal{J}(\lambda) = \sum_{h,k}\lambda_{hk}c_{hk} + \log\left[\sum_{\sigma}\exp\left\{-\sum_{h,k}\lambda_{hk}\sigma_h\sigma_k\right\}\right] \qquad (3.2.5)$$

Note that, $\nabla\mathcal{J} = 0$ implies $\mathcal{P}^*(\sigma)$ satisfies the constraints. A critical point exists if $\mathcal{J}$ is proper, which means,

$$\lim_{|\lambda|\to\infty}\mathcal{J}(\lambda) = +\infty$$

It is clear that the following set of inequalities ensure the properness of $\mathcal{J}$:

$$\sum_{i<j}c_{ij}\lambda_{ij} \geq \min\left\{\sum_{i<j}\lambda_{ij}\sigma_i\sigma_j : \sigma\in\Omega\right\} \text{ for every } \lambda$$

Let us denote by $M(\lambda)$ the minimum given by: $\min\left\{\sum_{i<j}\lambda_{ij}\sigma_i\sigma_j : \sigma\in\Omega\right\}$ and by Δ_n we denote the matrices satisfying the above set of inequalities:

$$\Delta_n = \left\{C = ((c_{ij})) : \sum_{i<j}c_{ij}\lambda_{ij} \geq M(\lambda) \text{ for every } \lambda\right\} \qquad (3.2.6)$$

Clearly, this is a "very large" set of inequalities. What do these inequalities signify and what do they tell us about covariance matrices of spins? We look at some specific inequalities among those determining the set Δ_n in the next section and analyze these inequalities in more detail.

3.3 Generalized Bell's inequalities

Let us first look at some of the inequalities that are satisfied by the matrices in the set Δ_n, as defined above in (3.2.6). We will see that for specific choices of λ_{ij}, these inequalities contain the inequalities that we have already seen to be necessary for C to be in Cov_n.

Proposition 3.3.1. *The set of inequalities that determine Δ_n contain the inequalities of positivity and Bell's inequalities*

Proof. 1. Positivity: Let $x \in \mathbb{R}^n$ and set $\lambda_{ij} = x_i x_j$. Then, for every $\sigma \in \Omega_n$

$$\sum_{ij} \lambda_{ij}\sigma_i\sigma_j = \sum_{ij} x_i x_j \sigma_i \sigma_j = \frac{1}{2}\left[\sum_i x_i \sigma_i\right]^2 \geq 0$$

So, $M(\lambda) \geq 0$. Thus, for $C \in \Delta_n$

$$\sum_{ij} x_i x_j c_{ij} \geq 0$$

which implies positivity.

2. Bell's inequalities: Let $A \subset \{1, 2, \ldots, n\}$ with $|A| = 3$, and $\varepsilon \in \{-1, 1\}^A$. We set

$$\lambda_{ij} = \begin{cases} \varepsilon_i \varepsilon_j & \text{for } \ i, j \in A, i \neq j \\ 0 & \text{otherwise} \end{cases}$$

Then, for $A = \{r, s, t\}$

$$\begin{aligned} \sum_{ij} \lambda_{ij}\sigma_i\sigma_j &= \varepsilon_r\varepsilon_s\sigma_r\sigma_s + \varepsilon_r\varepsilon_t\sigma_r\sigma_t + \varepsilon_s\varepsilon_t\sigma_s\sigma_t \\ &= \eta_r\eta_s + \eta_r\eta_t + \eta_s\eta_t \geq -1 \end{aligned}$$

where $\eta_i = \varepsilon_i\sigma_i$. So, we have $M(\lambda) \geq -1$. Thus, for $C \in \Delta_n$

$$\varepsilon_r\varepsilon_s c_{rs} + \varepsilon_r\varepsilon_t c_{rt} + \varepsilon_s\varepsilon_t c_{st} \geq -1$$

Or,

$$1 + \varepsilon_r\varepsilon_s c_{rs} + \varepsilon_r\varepsilon_t c_{rt} + \varepsilon_s\varepsilon_t c_{st} \geq 0$$

which are the Bell's inequalities.

□

In the above discussion, we have learned that the inequalities that determine the set Δ_n represent the feasibility conditions for the dual problem. That is, it is the H-representation of Cov_n. We prove this next:

Theorem 3.3.1. *Let Δ_n be as in defined in* (3.2.6) *and Cov_n be as defined in theorem 3.1.5. Then,*

$$\Delta_n = \mathrm{Cov}_n$$

Proof. We first show that $\Delta_n \subseteq \mathrm{Cov}_n$. Since Cov_n is closed, it is enough to show that $\overset{\circ}{\Delta}_n \subseteq \mathrm{Cov}_n$, where $\overset{\circ}{\Delta}_n$ denotes the interior of Δ_n. We know that,

$$\overset{\circ}{\Delta}_n = \left\{ C = ((c_{ij})) : \sum_{i<j} c_{ij}\lambda_{ij} > M(\lambda) \text{ for every } \lambda \right\}$$

Thus, for $C \in \overset{\circ}{\Delta}_n$, the dual functional $\mathcal{J}(\lambda)$ is proper. This implies feasibility. Thus, there exists a probability P that realizes C as a correlation matrix of spin variables. Hence $C \in \mathrm{Cov}_n$.

Now, to show $\mathrm{Cov}_n \subseteq \Delta_n$, let $C = ((c_{ij})) \in \mathrm{Cov}_n$. Then for every λ, we have

$$\begin{aligned}
\sum_{i,j} \lambda_{ij} c_{ij}^T &= E\left(\sum_{i,j} \lambda_{ij}\sigma_i\sigma_j \right) \\
&\geq \min_{\sigma} \sum_{i,j} \lambda_{ij}\sigma_i\sigma_j \\
&= M(\lambda)
\end{aligned}$$

This implies $C \in \Delta_n$

□

This gives us a complete set of inequalities that describe the set Cov_n. In the next chapter we will look at these inequalities more closely and see if we can exploit some properties and symmetries of λ_{ij} to obtain a minimal set of inequalities.

Now that we have seen in proposition 3.3.1, that the inequalities determining the set Δ_n contain certain knowns and essential inequalities, we look at these inequalities more closely. It is clear that with the "right" choice of λ, we can get some interesting inequalities. We explore this a little bit more. The basic questions is that of arriving at a minimal set of inequalities to describe Cov_n. For this, we need to understand the following:

- Can Δ_n be described by finitely many inequalities?
- How to obtain these inequalities?

We already know that Cov_n has 2^{n-1} extremals, and by theorem 3.3.1 we know that $\mathrm{Cov}_n = \Delta_n$, so it is clear that Δ_n can be described by a finite number of inequalities. It is however not trivial to

obtain these inequalities. We now look at some simple inequalities that can be obtained by choosing λ_{ij} in a particular way. In the following discussion, for the sake of notational convenience, we assume that the sum over i, j represents the sum over i, j such that $i < j$.

Let us consider $T \subset \{1, 2, \ldots, n\}$ such that $|T|$ is odd. Then, let $\varepsilon \in \{-1, 1\}^T$. We set,

$$\lambda_{ij} = \begin{cases} \varepsilon_i \varepsilon_j & \text{for } \ i, j \in T, i \neq j \\ 0 & \text{otherwise} \end{cases}$$

We have,

$$\sum_{i,j} \lambda_{ij} \sigma_i \sigma_j = \frac{1}{2} \left(\sum_{i \in T} \varepsilon_i \sigma_i \right)^2 - \frac{|T|}{2}$$

Since, $|T|$ is odd, therefore

$$\min_{\sigma} \left(\sum_{i \in T} \varepsilon_i \sigma_i \right)^2 = 1$$

We have, $M(\lambda) = \frac{1-|T|}{2}$. As a result, we obtain the inequality

$$\sum_{i,j} \lambda_{ij} c_{ij} = \sum_{i \neq j \in T} \varepsilon_i \varepsilon_j c_{ij} \geq \frac{1 - |T|}{2}$$

Or,

$$\frac{|T| - 1}{2} + \sum_{i,j} \lambda_{ij} c_{ij} \geq 0 \tag{3.3.1}$$

Notice that for $|T| = 3$, we obtain the Bell's inequalities from the above set of inequalities. We call (3.3.1), the Generalized Bell's inequalities. It turns out that (3.3.1) are in fact necessary and sufficient conditions for a matrix C of order $n = 5$ to be a spin correlation matrix. As we shall see later, a "good" choice of λ_{ij} leads us to the complete set of necessary and sufficient conditions for a 6×6 matrix to be a spin correlation matrix.

3.3.1 Some Explicit Examples

The program cdd+ (cdd, respectively) is a C++ (ANSI C) program for generating all vertices (i.e. extreme points) and extreme rays of a general convex polyhedron given by a system of linear inequalities:

$$P = \{x \in \mathbb{R}^d : Ax \leq b\}$$

where A is an $m \times d$ real matrix and b is a real m dimensional vector.

One useful feature of cdd/cdd+ is its capability of handling the dual problem without any transformation of data. The dual problem that is known as the convex hull problem and as we have discussed before it involves obtaining a linear inequality representation of a convex polyhedron given as the Minkowski sum of the convex hull of a finite set of points and the nonnegative hull of a finite set of points in $\mathbb{R}^d$: $P = conv(v_1, \ldots, v_n) + nonneg(r_1, \ldots, r_s)$, where the Minkowski sum of two subsets S and T of $\mathbb{R}^d$ is defined as $S + T = \{s + t | s \in S \text{ and } t \in T\}$.
We apply the cdd+ program for the cases $n = 5, 6$. We know the extremals in each from theorem 3.1.5. However, before looking at each case in details, we establish some notation.
Note that since each extremal is a correlation matrix, it is symmetric so we represent each matrix as a vector consisting of the upper-triangular entries listed row-wise. In other words, instead of considering the matrix $C = ((c_{ij}))_{1 \leq i,j \leq n}$, we consider the vector

$$v_C = (1, c_{12}, \ldots, c_{1n}, c_{2,3}, \ldots, c_{2,n}, \ldots, c_{n-1,n})$$

Thus, we transform the problem from the space of $n \times n$ matrices to vectors in $\mathbb{R}^N$ where $N = 1 + \frac{(n-1)n}{2}$. Note that, because of the symmetry of matrix we have only $\frac{(n-1)n}{2}$ relevant variables.

Example 6. *We first obtain the inequalities for the case n = 5. From theorem 3.1.5, we have* 16 *extremals given in the vector form by:*

$$\begin{aligned}
v_1 &= (1,1,1,1,1,1,1,1,1,1,1) \\
v_2 &= (1,-1,-1,-1,-1,1,1,1,1,1,1) \\
v_3 &= (1,1,-1,-1,-1,-1,-1,-1,1,1,1) \\
v_4 &= (1,-1,1,-1,-1,-1,1,1,-1,-1,1) \\
v_5 &= (1,-1,-1,1,-1,1,-1,1,-1,1,-1) \\
v_6 &= (1,-1,-1,-1,1,1,1,-1,1,-1,-1) \\
v_7 &= (1,1,1,-1,-1,1,-1,-1,-1,-1,1) \\
v_8 &= (1,1,-1,1,-1,-1,1,-1,-1,1,-1) \\
v_9 &= (1,1,-1,-1,1,-1,-1,1,1,-1,-1) \\
v_{10} &= (1,-1,1,1,-1,-1,-1,1,1,-1,-1) \\
v_{11} &= (1,-1,1,-1,1,-1,1,-1,-1,1,-1) \\
v_{12} &= (1,-1,-1,1,1,1,-1,-1,-1,-1,1) \\
v_{13} &= (1,-1,1,1,1,-1,-1,-1,1,1,1) \\
v_{14} &= (1,1,-1,1,1,-1,1,1,-1,-1,1) \\
v_{15} &= (1,1,1,-1,1,1,-1,1,-1,1,-1) \\
v_{16} &= (1,1,1,1,-1,1,1,-1,1,-1,-1)
\end{aligned}$$

In the corresponding H-representation, we have 56 *inequalities in* 10 *variables, namely,* $c_{12}, c_{13}, c_{14}, c_{15}, c_{23}, c_{24}, c_{25}, c_{34}, c_{35}, c_{45}$. *The inequalities are given by*

$$M\check{c} \geq \vec{0}$$

where $\check{c} = (1, c_{12}, c_{13}, c_{14}, c_{15}, c_{23}, c_{24}, c_{25}, c_{34}, c_{35}, c_{45})$ *is a* 11×1 *vector and* M *is a* 56×11 *matrix given by*

$$M = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\
1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \\
1 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\
2 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \\
2 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 \\
2 & 1 & -1 & 1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 \\
2 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 \\
1 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
2 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
2 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 \\
1 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \\
2 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & -1 & 1 \\
2 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 \\
2 & -1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 \\
2 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 \\
2 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\
2 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\
2 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\
2 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 \\
2 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 \\
2 & -1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\
1 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & -1 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 \\
1 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & -1 \\
1 & 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 & -1 & 0 \\
1 & 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 \\
1 & 1 & 0 & 0 & -1 & 0 & 0 & -1 & 0 & 0 & 0 \\
1 & 1 & 0 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & -1 & 0 & 0 \\
1 & 1 & -1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & -1 & -1 & 0 & 1 & 0 & 0 \\
1 & 0 & -1 & -1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & -1 & 0 & 0 \\
1 & -1 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
1 & -1 & 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\
1 & -1 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
1 & -1 & -1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 & -1 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & -1 \\
1 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & -1 \\
1 & 0 & 0 & 0 & 0 & -1 & 0 & 1 & 0 & -1 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & 1 \\
1 & 0 & -1 & 0 & 1 & 0 & 0 & 0 & 0 & -1 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & 1 \\
1 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 1 & 0 \\
1 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0 \\
1 & -1 & 0 & 0 & -1 & 0 & 0 & 1 & 0 & 0 & 0 \\
1 & -1 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & 0
\end{pmatrix}$$

There are precisely 16 *inequalities with constant term* 2*, corresponding to the inequalities that come from taking* $|T| = 5$ *in the generalized Bell's inequalities obtained in previous section. The rest* 40 *come from the inequalities obtained by taking* $|T| = 3$*. In fact these are exactly the same inequalities. This is easy to see. Given three variables* (c_{ij}, c_{kl}, c_{rs})*, we get* 4 *different inequalities from the generalized Bell's inequalities* (3.3.1) *(these are the original Bell's inequalities). Then, for all* T *such that* $|T| = 3$*, there are exactly* $\binom{5}{3} \times 4 = 40$ *inequalities.*

Example 7. *For n = 6, we have* 32 *extremals given by:*

$$
\begin{aligned}
v_1 &= (1,1,1,1,1,1,1,1,1,1,1,1,1,1,1,1)\\
v_2 &= (1,-1,1,1,1,1,-1,-1,-1,-1,1,1,1,1,1,1)\\
v_3 &= (1,1,-1,1,1,1,-1,1,1,1,-1,-1,-1,1,1,1)\\
v_4 &= (1,1,1,-1,1,1,1,-1,1,1,-1,1,1,-1,-1,1)\\
v_5 &= (1,1,1,1,-1,1,1,1,-1,1,1,-1,1,-1,1,-1)\\
v_6 &= (1,1,1,1,1,-1,1,1,1,-1,1,1,-1,1,-1,-1)\\
v_7 &= (1,-1,-1,1,1,1,1,1,-1,-1,-1,-1,-1,-1,1,1,1,1)\\
v_8 &= (1,1,-1,-1,1,1,-1,-1,1,1,1,-1,-1,-1,-1,1)\\
v_9 &= (1,1,1,-1,-1,1,1,-1,-1,1,-1,-1,1,1,-1,-1)\\
v_{10} &= (1,1,1,1,-1,-1,1,1,-1,-1,1,-1,-1,-1,-1,1)\\
v_{11} &= (1,-1,1,-1,1,1,-1,1,-1,-1,-1,1,1,-1,-1,1)\\
v_{12} &= (1,-1,1,1,-1,1,-1,-1,1,-1,1,-1,1,-1,1,-1)\\
v_{13} &= (1,-1,1,1,1,-1,-1,-1,-1,1,1,1,-1,1,-1,-1)\\
v_{14} &= (1,1,-1,1,-1,1,-1,1,-1,1,-1,1,-1,-1,1,-1)\\
v_{15} &= (1,1,-1,1,1,-1,-1,1,1,-1,-1,-1,1,1,-1,-1)\\
v_{16} &= (1,1,1,-1,1,-1,1,-1,1,-1,-1,1,-1,-1,1,-1)\\
v_{17} &= (1,-1,-1,1,-1,-1,1,-1,1,1,-1,1,1,-1,-1,1)\\
v_{18} &= (1,-1,-1,-1,1,-1,1,1,-1,1,1,-1,1,-1,1,-1)\\
v_{19} &= (1,-1,1,-1,-1,-1,-1,1,1,1,-1,-1,-1,1,1,1)\\
v_{20} &= (1,-1,-1,-1,-1,1,1,1,1,-1,1,1,-1,1,-1,-1)\\
v_{21} &= (1,1,-1,-1,-1,-1,-1,-1,-1,-1,1,1,1,1,1,1)\\
v_{22} &= (1,-1,-1,-1,1,1,1,1,-1,-1,1,-1,-1,-1,-1,1)\\
v_{23} &= (1,1,-1,-1,-1,1,-1,-1,-1,1,1,1,-1,1,-1,-1)\\
v_{24} &= (1,1,1,-1,-1,-1,1,-1,-1,-1,-1,-1,-1,1,1,1)\\
v_{25} &= (1,-1,1,-1,1,-1,-1,1,-1,1,-1,1,-1,-1,1,-1)\\
v_{26} &= (1,-1,-1,1,-1,1,1,-1,1,-1,-1,1,-1,-1,1,-1)
\end{aligned}
$$

$$v_{27} = (1,-1,-1,1,1,-1,1,-1,-1,1,-1,-1,1,1,-1,-1)$$
$$v_{28} = (1,1,-1,-1,1,-1,-1,-1,1,-1,1,-1,1,-1,1,-1)$$
$$v_{29} = (1,-1,1,1,-1,-1,-1,-1,1,1,1,-1,-1,-1,-1,1)$$
$$v_{30} = (1,-1,1,-1,-1,1,-1,1,1,-1,-1,-1,1,1,-1,-1)$$
$$v_{31} = (1,1,-1,1,-1,-1,-1,1,-1,-1,-1,1,1,-1,-1,1)$$
$$v_{32} = (1,-1,-1,-1,-1,-1,1,1,1,1,1,1,1,1,1,1)$$

The corresponding inequalities are again given by

$$M\check{c} \geq \vec{0}$$

where, $\check{c} = (1, c_{12}, c_{13}, c_{14}, c_{15}, c_{16}, c_{23}, c_{24}, c_{25}, c_{26}, c_{34}, c_{35}, c_{36}, c_{45}, c_{46}, c_{56})$ *is a* 16×1 *vector and* M *is a* 368×16 *matrix.*

There are 80 *inequalities with constant term* 1*,* 96 *inequalities with constant term* 2 *and remaining* 192 *with constant term* 4*. The first two set of inequalities are exactly the Generalized Bell's inequalities for* $|T| = 3$ *(number of inequalities* $= 2^2 \times \binom{6}{3} = 80$*) and for* $|T| = 5$ *(number of inequalities* $= 2^4 \times \binom{6}{5} = 96$*).*

Where do the remaining 192 *inequalities come from?*

We go back to Theorem 3.3.1. It is clear that we essentially need to find a suitable choice of λ_{ij}*. Recall the derivation of Generalized Bell's inequalities of section 3.3. Following the same notation, we consider* $T \subset \{1, 2, \ldots, n\}$ *such that* $|T| = 5$*. Then, let* $\varepsilon \in \{-1, 1\}^T$*. We set,*

$$\lambda_{ij} = \begin{cases} \varepsilon_i \varepsilon_j & \text{for } \ i, j \in T, i \neq j \\ 2\epsilon_i \epsilon_j & \text{when either } i \text{ or } j \ \notin T \end{cases}$$

Or,

$$\lambda_{ij} = \begin{cases} \varepsilon_i \varepsilon_j & \text{for } \ i, j \in T, i \neq j \\ 2\epsilon_i \epsilon_k & \text{for } i \in T, k \notin T \end{cases} \tag{3.3.2}$$

Notice that this gives us precisely 15 λ'_{ij}*s.*

We have seen that,

$$\sum_{i,j \in T} \lambda_{ij} \sigma_i \sigma_j = \frac{1}{2} \left(\sum_{i \in T} \varepsilon_i \sigma_i \right)^2 - \frac{|T|}{2}$$

Thus,

$$M(\lambda) = \min_{\sigma} \left\{ \sum_{ij} \sigma\sigma_j \lambda_i j \right\}$$

$$= \min_{\sigma} \left\{ \frac{1}{2} \left(\sum_{i \in T} \varepsilon_i \sigma_i \right)^2 - \frac{|T|}{2} + 2 \left(\sum_{i \in T} \varepsilon_i \varepsilon_k \sigma_i \sigma_k \right) \right\} \tag{3.3.3}$$

$$= \min_{\sigma} \left\{ \frac{1}{2} \left(\sum_{i \in T} \varepsilon_i \sigma_i \right)^2 - \frac{|T|}{2} + 2\varepsilon_k \sigma_k \left(\sum_{i \in T} \varepsilon_i \sigma_i \right) \right\} \tag{3.3.4}$$

$$= \min_{\sigma} \left\{ \frac{1}{2} \left(\sum_{i \in T} \varepsilon_i \sigma_i \right)^2 - \frac{|T|}{2} \pm 2\sigma_k \left(\sum_{i \in T} \varepsilon_i \sigma_i \right) \right\} \tag{3.3.5}$$

Since, $|T| = 5$ *we have,*

$$M(\lambda) = \min_{\sigma} \left\{ \frac{1}{2} \left(\sum_{i \in T} \varepsilon_i \sigma_i \right)^2 \pm 2\sigma_k \left(\sum_{i \in T} \varepsilon_i \sigma_i \right) - \frac{5}{2} \right\}$$

We need to find the minimum of the function $\frac{1}{2}x^2 \pm 2\sigma_k x - \frac{5}{2}$*, where* x *takes values* $\pm 1, \pm 3, \pm 5$*. It turns out that,*

$$M(\lambda) = -4$$

$$\sum_{i,j} \lambda_{ij} c_{ij} \geq M(\lambda) = -4$$

This gives us $2^5 \times \binom{6}{5} = 192$ *inequalities given by*

$$4 + \sum_{i,j} \lambda_{ij} c_{ij} \geq 0 \tag{3.3.6}$$

where λ_{ij} *are as defined in* (3.3.2)*. These are precisely the inequalities obtained by cdd+.*

3.3.2 The Translation Invariant Case

Let us now look at some special cases where we introduce some geometrical structure on the spin system. Assume that the spins $(\sigma_1, \ldots, \sigma_n)$ are lying on a circle and that the distance between σ_i and σ_j is given by $|i - j|$ modulo n. We assume that the correlation matrix is translation invariant. That is, $c_{ij} = c_{hk}$ if $|i - j| = |h - k|$ (modulo n).

In this case, the correlation matrix is of the form

$$\begin{pmatrix} 1 & a & b & \dots & b & a \\ a & 1 & a & b & \dots & b \\ b & \dots & 1 & a & b & \dots \\ \dots & b & a & 1 & a & b \\ b & \dots & b & a & 1 & a \\ a & b & \dots & b & a & 1 \end{pmatrix}$$

That is, each off-diagonal is constant and the corresponding inner and outer off-diagonals are equal. Thus is this case we only have $\frac{n(n-1)}{4}$ or $1 + \frac{n(n-2)}{4}$ variables depending on whether $\frac{n(n-1)}{2}$ is even or odd respectively.

We represent this set of variables by $\check{c} = (c_1, c_2, \dots, c_N)$. Then, we want to find a matrix M such that $M\check{c} \geq 0$ gives the H-representation of Cov_n. We will find the explicit inequalities for $n = 5$ and 6 and then analyze them to see how they fit into the set of Generalized Bell's inequalities.

However, we don't have description of set of correlation matrices in terms of extremals for the translation invariant case. We have the complete set of inequalities for $n = 5$ and 6. In each case we can add the equalities to this set and then use cdd+ to solve the dual problem (the vertex enumeration problem) and thus obtain the extremals for the translation invariant case. For instance, we can find the set of extremals in the case of $n = 5$ by adding equalities $c_{12} = c_{23} = c_{34} = c_{45} = c_{15}$ and $c_{13} = c_{25} = c_{35} = c_{14} = c_{25}$ to the 56 inequalities from example (1.1). We then run cdd+ to solve the facet enumeration problem, to get the necessary and sufficient inequalities, starting from this new set of extremals.

Example 8. *For n = 5, in the translation invariant case, we have three extremals*

$$\begin{aligned} v_1 &= (1, 1, 1) \\ v_2 &= (1, -3/5, 1/5) \\ v_3 &= (1, 1/5, -3/5) \end{aligned}$$

Then, the corresponding H-representation is given by

$$\begin{pmatrix} 1 & -2 & 1 \\ 1 & 1 & -2 \\ 1 & 5/2 & 5/2 \end{pmatrix} \begin{pmatrix} 1 \\ c_1 \\ c_2 \end{pmatrix} \geq \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Example 9. *For $n = 6$, in the translation invariant case, we follow the same procedure as in the case of $n = 5$ and obtain six extremals*

$$\begin{aligned} v_1 &= (1, 1, 1, 1) \\ v_2 &= (1, -1/3, -1/3, 1) \\ v_3 &= (1, 1/3, -1/3, -1/3) \\ v_4 &= (1, -1/3, -1/3, 1/3) \\ v_5 &= (1, 1/3, -1/3, -1) \\ v_6 &= (1, -1, 1, -1) \end{aligned}$$

Then, the corresponding H-representation is given by

$$\begin{pmatrix} 1 & 0 & 3 & 0 \\ 1 & 2 & 1 & 0 \\ 1 & 2 & 2 & 1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -2 & 2 & -1 \\ 1 & -2 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ c_1 \\ c_2 \\ c_3 \end{pmatrix} \geq \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

After analyzing the necessary and sufficient conditions obtained above, one concludes that the above inequalities are a subset of (3.3.1) and the inequalities obtained in (3.3.6) don't contribute anything in this case.

Thus, for the stationary case for both $n = 5$ and 6, the generalized Bell's inequalities are necessary and sufficient.

Chapter 4

An Explicit Solution for Spin Covariance Realization Problem

4.1 Georgiou's Theorem

In this chapter we will look at the second part of the problem, namely, given a matrix of spin correlations, how does one explicitly find a measure that realizes the given correlations. Tryphon T. Georgiou's paper [14] discusses this problem in great generality. We first look at the method described in his paper in detail and then look at the specific case of spin systems and give a method to explicitly find the required measure.

4.1.1 Setting

Let us consider $\mathbb{R}^n$ with the usual inner product, i.e., for $x, y \in \mathbb{R}^n$:

$$\langle x, y \rangle = \sum_{i=1}^{n} x_i y_i$$

We will be dealing with the following problem. Let $S \subseteq R^m$ be the cartesian product of m closed intervals, and $G : R^m \longrightarrow R^k$, where $m, k \geq 1$. Given $R \in R^k$, the aim is to identify, if any, all positive measures μ on S such that $\int G(\theta) d\mu(\theta) = R$. Note that if we set one component of G equal to 1 as well as the corresponding component of R, one restricts to probability measures. Later we will consider the case in which S is a finite set, that can be dealt with similarly.

The idea is to trace a path in the space of Lagrange multipliers (denoted by λ) by following a

path homotopy in the moment space. A differential equation involving the Lagrange multipliers is obtained. The differential equation converges to the "right" vector of Lagrange multipliers if the moment problem is solvable i.e. the moments are realizable, otherwise, it diverges. Thus, the method also provides an independent way to test the feasibility of given moments. In fact, the method is employed to characterize the complete solution set of positive measures that realize the given moments.

Let $S \subseteq \mathbb{R}^m (m \in \mathbb{N})$ be the cartesian product of m closed intervals as defined above. Let $(g_0, g_1, , \ldots, g_N)$ be linearly independent continuous measurable functions from S to $\mathbb{R}$. Then, we define $G : S \longrightarrow R^N$ as $G : \theta \mapsto [g_0(\theta), \ldots, g_N(\theta)]$ for $\theta \in S$. Define by $\mathfrak{G} = \{G(\theta) : \theta \in S\}$ a surface in $\mathbb{R}^{N+1}$.

Consider the *closed conic hull* of $\mathfrak{G}$ by:

$$\mathfrak{R}(\mathfrak{G}) = \{R : R = \sum_{i=1}^{K} G(\theta_i)\alpha_i \quad \forall\, \theta_i \in \mathcal{S}, \alpha_i \in \mathbb{R}, \alpha_i > 0, K = 1, 2, \ldots\}$$

and the dual cone by:

$$\mathfrak{R}_+^*(\mathfrak{G}) = \{\lambda \in \mathbb{R}^N : \langle \lambda, R\rangle \geq 0 \quad \forall \;\; R \in \mathfrak{R}(\mathfrak{G})\}$$

The dual cone $\mathfrak{R}_+^*$ represents the cone of all vectors λ in the dual space $(\mathbb{R}^N)^*$ which form an acute or right angle with any vector of $\mathfrak{R}$.

Remark 4.1.1. It is easy to see that λ is an interior point of $\mathfrak{R}_+^*(\mathfrak{G})$ if and only if $\langle \lambda, G\rangle$ is strictly positive on S.

Theorem 4.1.1. *The cone $\mathfrak{R}(\mathfrak{G})$ is the set of points R such that*

$$R = \int_S G(\theta) d\mu(\theta) \tag{4.1.1}$$

where μ is a non-negative measure on S.

We denote the set of all nonnegative Borel measures on S by $\mathcal{M}$. Note that this is a closed convex cone.

Then, we want to know, for a given $R \in \mathbb{R}^{N+1}$,

- Does there exist a measure $\mu \in \mathcal{M}$ such that (4.1.1) holds?
- If yes, then what are all the μ's that satisfy this?

In [14], following families of measures is considered:

$$\mathcal{M}_{rat} = \left\{ \frac{\Psi(\theta)}{\langle \lambda, G(\theta)\rangle} d\theta \right\}$$
$$\mathcal{M}_{exp} = \left\{ \Psi(\theta) e^{-\langle \lambda, G(\theta)\rangle} d\theta \right\}$$

where $\Psi > 0$ is an arbitrary but fixed function that allows us to span the whole set of positive measures that are consistent with the given moments. As we will see, the convergence (and divergence

resp.) of the differential equation constructed does not depend on Ψ. In the following discussion we will only consider the exponential family $\mathcal{M}_{exp}$ (which is relevant to the context of this thesis), the discussion and proofs of for the rational case are similar and can be found in [14]. We discuss the case of the exponential family in detail and reproduce the proofs.

4.1.2 Main Theorem

The main theorem of [14] gives the differential equation for the Lagrange multipliers. This is done in the paper for a closed interval ($S \subset \mathbb{R}^m$). Since, we will be considering this theorem in the context of spin systems here, we reproduce the statement and the proof for S discrete. The proof is essentially the same. We are considering here the family of discrete measure given by

$$\mathcal{M}_{exp} = \{\Psi(\sigma)e^{-\langle\lambda,G(\sigma)\rangle}\}$$

The rest of the discussion follows through once the integrals are replaced by sums.

Theorem 4.1.2. *Let $S, G, \mathcal{G}, \Psi$ be as above. Consider $R_1 \in \mathbb{R}^{N+1}$. Consider the differential equation -*

$$\frac{d\lambda(t)}{dt} = -M(\lambda)^{-1}\left(R_1 - \sum_S G(\sigma)\Psi(\sigma)e^{-\langle\lambda,G(\sigma)\rangle}\right) \tag{4.1.2}$$

where,

$$M(\lambda) = \sum_S G(\sigma)\Psi(\sigma)e^{-\langle\lambda,G(\sigma)\rangle}G(\sigma)^T$$

and $\lambda(0) = \lambda_0$.

Note that $G(\sigma)^T$ denotes the transpose of the column vector $G(\sigma)$. If $R_1 \in$ int $(\mathfrak{R}(\mathfrak{G}))$, then as $t \longrightarrow \infty$ the solution $\lambda(t)$ of the differential equation tends to a limit λ_1 so that the measure $\Psi(\sigma)e^{-\langle\lambda_1,G(\sigma)\rangle} \in \mathcal{M}_{exp}$ satisfies

$$R_1 = \sum_S G(\sigma)\Psi(\sigma)e^{-\langle\lambda_1,G(\sigma)\rangle} \tag{4.1.3}$$

Moreover the following hold:

1. *The trajectory $\{\lambda(t) : t \in [0,\infty)\}$ remains bounded.*
2. *The limit point λ_1 is the unique solution of* (4.1.2) *in $\mathbb{R}^N$*

Conversely, if $R_1 \notin$ int $(\mathfrak{R}(\mathfrak{G}))$, then $\|\lambda(t)\| \longrightarrow \infty$.

Consider a path from R_0 to R_1 given by: $R_\rho = (1-\rho)R_0 + \rho R_1$, (where $\rho \in [0,1]$). We then consider the family of equations

$$R_\rho = \sum_S G(\sigma)\mu_\rho(\sigma)$$

where $\rho \in [0,1]$. This links μ_0 to the sought-after solution μ_1 (parametrized by the corresponding λ_1).

We look at the one-parameter homotopy

$$H(\rho,\lambda) = \sum_S G(\sigma)\mu_\rho(\sigma,\lambda) - R_\rho = 0 \tag{4.1.4}$$

Note that $H(1,\lambda) = 0$ is equivalent to

$$R_1 = \sum_S G(\sigma)\mu(\sigma,\lambda_1) \tag{4.1.5}$$

for which we want to find a solution, and $H(0,\lambda) = 0$ is equivalent to

$$R_0 = \sum_S G(\sigma)\mu(\sigma,\lambda_0) \tag{4.1.6}$$

for which the solution is known.

If the equation $H(\rho,\lambda) = 0$ has a solution $\lambda(\rho)$, such that

$$\frac{\partial H(\rho,\lambda)}{\partial \lambda}$$

is non-singular at $(\rho,\lambda(\rho))$ for $\rho \in [0,1]$, then it follows from the Implicit function theorem that $\lambda(\rho)$ satisfies the differential equation

$$\frac{d\lambda(\rho)}{d\rho} = -\left(\frac{\partial H(\rho,\lambda)}{\partial \lambda}\right)^{-1} \frac{\partial H(\rho,\lambda)}{\partial \rho} \tag{4.1.7}$$

with $\lambda(0) = \lambda_0$.

Conversely, if the above differential equation has a solution $\lambda(\rho)$ for $\rho \in [0,1]$, then $\frac{dH(\rho,\lambda(\rho))}{d\rho} = 0$ for $\rho \in [0,1]$. Therefore, $H(1,\lambda_1) = H(0,\lambda_0) = 0$. From λ_1 we get the corresponding μ_1 that gives the vector of moments given by R_1.

Let us calculate $\frac{\partial H(\rho,\lambda)}{\partial \lambda}$ and $\frac{\partial H(\rho,\lambda)}{\partial \rho}$, to understand the differential equation in (4.1.7).

It is clear that $\frac{\partial H(\rho,\lambda)}{\partial \rho} = R_0 - R_1$. The partial derivative of $H(\rho,\lambda)$ with respect to λ for $\mu_\rho(\sigma,\lambda) = \sum_S G(\sigma)\Psi(\sigma)e^{-\langle\lambda,G(\sigma)\rangle}$ is given by,

$$\frac{\partial H(\rho,\lambda)}{\partial \lambda} = -\sum_S G(\sigma)\Psi(\sigma)e^{-\langle\lambda,G(\sigma)\rangle}G(\sigma)^T = -M(\lambda)$$

Now, changing the variables, $\rho = 1 - e^{-t}$ and substituting $R_1 - R_0 = \frac{1}{\rho - 1}(R_1 - R_\rho)$, we get -

$$\begin{aligned}
\frac{d\lambda(t)}{dt} &= -\left(\frac{\partial H(\rho,\lambda)}{\partial \lambda}\right)^{-1} \frac{\partial H(\rho,\lambda)}{\partial \rho} \\
&= -\left(\frac{\partial H(\rho,\lambda)}{\partial \lambda}\right)^{-1} (R_0 - R_1)(1-\rho) \\
&= -\left(\frac{\partial H(\rho,\lambda)}{\partial \lambda}\right)^{-1} (R_\rho - R_1) \\
&= M(\lambda)^{-1}(R_\rho - R_1)
\end{aligned}$$

We will show that $M(\lambda)$ is bounded and invertible along the trajectories of (4.1.7) for all $\rho \in [0,1]$, if and only if , $R_1 \in \text{int}(\mathfrak{R}(\mathfrak{G}))$.

We now prove the theorem.

Proof. Consider

$$\frac{d\lambda(t)}{d\rho} = -M(\lambda)^{-1}(R_1 - R_0) \tag{4.1.8}$$

where $M(\lambda) = \sum_S G(\sigma)\Psi(\sigma)e^{-\langle \lambda, G(\sigma)\rangle}G(\sigma)^T$.

Note that the vector G consists of linearly independent functions on S and $e^{\langle \lambda, G\rangle}$ is positive and bounded along the trajectories of (4.1.8). So, $M(\lambda)$ is bounded and nonsingular along the trajectories of (4.1.8). It follows that we can integrate (4.1.8) over a maximal interval $[0, \epsilon)$.

Now if $\epsilon > 1$, it means that the above differential equation has a solution $\lambda(\rho)$ for $\rho \in [0,1]$. This implies (as discusses before), $\frac{dH(\rho,\lambda(\rho))}{d\rho} = 0$ for $\rho \in [0,1]$. So, $H(1,\lambda_1) = H(0,\lambda_0) = 0$. Let $\mu_1 = \psi(\sigma)e^{-\langle \lambda_1, G(\sigma)\rangle}$ which is a positive measure. Then, this μ_1 satisfies -

$$R_1 = \sum_S G(\sigma)\mu(\sigma,\lambda) \tag{4.1.9}$$

Hence, by theorem 4.1.1, $R_1 \in \text{int}(\mathfrak{R}(\mathfrak{G}))$.

Conversely, if $\epsilon < 1$ ie. $M(\lambda)$ is not bounded. We want to prove that in this case, $R_1 \notin int(\mathfrak{R}(\mathfrak{G}))$.

We know that, $M(\lambda)$ is not bounded outside $[0,\epsilon)$ (i.e, $\|d\lambda(\rho)/d\rho\|$ ans $\|\lambda(\rho)\|$ increase without bound) means $\sum_S G(\sigma)\Psi(\sigma)e^{-\langle \lambda, G(\sigma)\rangle}G(\sigma)^T$ blows up as $\rho \longrightarrow \epsilon$.

We will show that $R_\epsilon \notin int(\mathfrak{R}(\mathfrak{G}))$

Consider a convergent sequence $\alpha_i = \lambda(\rho_i)/\|\lambda(\rho_i)\|$ for suitably selected $\rho_i \in [0,\epsilon)$ such that as $\rho_i \longrightarrow \epsilon$, $\alpha_i \longrightarrow \alpha$.

Claim 4.1.1. *α is a boundary point of $\mathfrak{R}^*_+(\mathfrak{G})$.*

Proof. Consider -

$$\sum_S G(\sigma)\Psi(\sigma)e^{-\langle\lambda(\rho_i),G(\sigma)\rangle} = \sum_S G(\sigma)\Psi(\sigma)e^{-\|\lambda(\rho_i)\|\langle\alpha_i,G(\sigma)\rangle} \longrightarrow R_\epsilon$$

If $\alpha \notin \mathfrak{R}^*_+(\mathfrak{G})$, then for i large enough, $\langle\alpha_i, G(\sigma)\rangle < 0$ on a non-empty subset of S. We know that $\|\lambda(\rho_i)\| \longrightarrow \infty$. This would imply that the above sum blows up which is a contradiction.

Now if $\alpha \in int(\mathfrak{R}^*_+(\mathfrak{G}))$, then for large enough i, $\langle\alpha_i, G(\sigma)\rangle > 0$ on S (Remark 4.1.1). This along with the fact that $\|\lambda(\rho_i)\| \longrightarrow \infty$ would imply that the above sum would tend to 0, which again is a contradiction. □

This means $\langle\alpha, G\rangle \geq 0$ on S (It vanishes on a subset S_0 of S such that $S_0 \neq \varphi$ or S).

So we know that α is on the boundary $\mathfrak{R}^*_+(\mathfrak{G})$ and a sequence α_i converges to α from the $int(\mathfrak{R}^*_+(\mathfrak{G}))$ (as $\rho_i \longrightarrow \epsilon$ in $[0, \epsilon)$) such that correspondingly the sums R_{ρ_i} converge to R_ϵ.
Now to show that $R_\epsilon \notin int(\mathfrak{R}(\mathfrak{G}))$, it is enough to prove that $\langle\alpha, R_{\rho_i}\rangle \longrightarrow 0$ as $i \longrightarrow \infty$

$$\begin{aligned}\langle\alpha, R_{\rho_i}\rangle &= \langle\alpha, \sum_S G(\sigma)\Psi(\sigma)e^{-\|\lambda(\rho_i)\|\langle\alpha_i,G(\sigma)\rangle}\rangle \\ &= \langle\alpha, \sum_{S_0} G(\sigma)\Psi(\sigma)e^{-\|\lambda(\rho_i)\|\langle\alpha_i,G(\sigma)\rangle}\rangle + \langle\alpha, \sum_{S\setminus S_0} G(\sigma)\Psi(\sigma)e^{-\|\lambda(\rho_i)\|\langle\alpha_i,G(\sigma)\rangle}\rangle\end{aligned}$$

Now, we know that α vanishes on S_0 and is strictly positive outside i.e. on $S \setminus S_0$. But from the discussion above we know that on $S \setminus S_0$,

$$\sum G(\sigma)\Psi(\sigma)e^{-\|\lambda(\rho_i)\|\langle\alpha_i,G(\sigma)\rangle} \longrightarrow 0$$

Thus, $\langle\alpha, R_{\rho_i}\rangle \longrightarrow 0$ as $i \longrightarrow \infty$. This implies $R_\epsilon \notin int(\mathfrak{R}(\mathfrak{G}))$ which implies that $R_1 \notin int(\mathfrak{R}(\mathfrak{G}))$ because of the convexity of $\mathfrak{R}(\mathfrak{G})$ and the fact that $R_0 \in int(\mathfrak{R}(\mathfrak{G}))$.

We now prove the uniqueness.

We denote by h the map $\lambda \mapsto R = \sum_S G(\sigma)\mu(\lambda, \sigma)$. Suppose there exist two distinct λ_1 and λ_2 that give the same $R' \in int(\mathfrak{R}(\mathfrak{G}))$. Consider the path $(1-\rho)\lambda_1 + \rho\lambda_2$, for $\rho \in [0, 1]$. Denote the corresponding moment vector by R_ρ (i.e. $R_\rho = h(\lambda_\rho)$). Note that $R_0 = R_1 = R'$. This means $(\int_0^1 (\partial h/\partial\lambda)d\rho)(\lambda_2 - \lambda_1) = 0$ but this is a contradiction because $\partial h/\partial\lambda = -\sum_S G(\sigma)\mu(\lambda, \sigma)G(\sigma)^T$ is negative-definite throughout. (Note that: for any $x \in \mathbb{R}^N$, we have, $x^T G(\sigma)G(\sigma)^T x = (x^T G(\sigma))^2$). This implies $\lambda_1 = \lambda_2$.

□

We have shown that the differential equation converges to a unique λ that is in fact the parameter matrix of the measure that realizes the given moments. We will now prove that the convergence is in fact Lyapunov.

Proposition 4.1.1. *The function*

$$V(\lambda) = \|R_1 - \sum_{\sigma \in S} G(\sigma) m(\lambda, \sigma)\|^2$$

is a Lyapunov function for the differential equation $\frac{d\lambda}{dt} = f(\lambda)$ *(where* $\|.\|$ *is the usual Euclidean norm in* $\mathbb{R}^{N+1}$ *). Moreover, along the trajectories, it holds that*

$$\frac{V(\lambda(t))}{dt} = -2V(\lambda(t))$$

Proof. Clearly, V is continuous, differentiable with $V(\lambda) \geq 0$ for $\lambda \in \mathbb{R}^{N+1}$ and only vanishes at the fixed point of $\frac{d\lambda}{dt} = f(\lambda)$. We have,

$$\frac{d\lambda}{dt} = \left(\frac{\partial R}{\partial \lambda}\right)^{-1} \left(R_1 - \sum_{\sigma \in S} G(\sigma) m(\lambda, \sigma)\right)$$

Hence,

$$\begin{aligned}
\frac{dV(\lambda(t))}{dt} &= \left(\frac{\partial R}{\partial \lambda}\right)^{-1} \left(R_1 - \sum_{\sigma \in S} G(\sigma) m(\lambda, \sigma)\right) \\
&= -2 \left(R_1 - \sum_{\sigma \in S} G(\sigma) m(\lambda, \sigma)\right)' \left(\frac{\partial R}{\partial \lambda}\right) \frac{d\lambda}{dt} \\
&= -2 \left(R_1 - \sum_{\sigma \in S} G(\sigma) m(\lambda, \sigma)\right)' \times \left(R_1 - \sum_{\sigma \in S} G(\sigma) m(\lambda, \sigma)\right) \\
&= -2V(\lambda(t))
\end{aligned}$$

□

So, if R_1 is realizable, that is, it admits the representation (4.1.1), then the differential equation of theorem 4.1.2 converges to a point say λ_0 and one can find a positive measure μ_0 parametrized by λ_0 that realizes R_1.

4.2 Spin Systems

We consider the application of this method in the special case of spin variables. We keep the earlier notation. So, $\Omega_n = \{-1, 1\}^n$ denotes the space of length-n sequences which are denoted by $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_n)$, where each $\sigma_i \in \{-1, 1\}$ is a spin variable.

We are given the spin-spin correlations, $c_{ij} := E(\sigma_i\sigma_j)$ (with $E(\sigma_i) \equiv 0$ for all $1 \leq i \leq n$), and we want to find a probability measure that realizes these correlations.

In the notation of Chapter 3, $S = \Omega_n$. The set $\{g_0, g_1, \ldots, g_N\}$ is defined as follows:

$$g_0 \equiv 1 \text{ and } g_{ij}(\sigma) = \sigma_i\sigma_j \text{ where } 1 \leq i < j \leq n$$

and $N = \frac{n(n-1)}{2}$

$$\mathfrak{G} = \{G(\sigma) : \sigma \in \mathcal{S}\} \subset \{-1, 1\}^{N+1} \subset \mathbb{R}^{N+1}$$

$\mathfrak{R}_+(\mathfrak{G})$ and $\mathfrak{R}^*_+(\mathfrak{G})$ are as defined in the previous section.

Note that, one of the essential conditions for the main theorem to follow is that the set of functions $\{g_0, g_1, \ldots, g_N\}$ are linearly independent. We prove this for the case of spins now.

Lemma 4.2.1. *The set of functions* $\{g_{ij}(\sigma) = \sigma_i\sigma_j\} \cup \{g_0\}$ *where* $1 \leq i < j \leq n$ *are linearly independent.*

Proof. Consider a linear combination

$$\sum_{i<j} \alpha_{ij} g_{ij} + \alpha_0 g_0 = 0$$

This means,

$$\sum_{j\neq 1} \alpha_{1,j}\sigma_1\sigma_j + \sum_{i<j, i\neq 1} \alpha_{ij} g_{ij} + \alpha_0 = 0$$

Or,

$$\sigma_1 \sum_{j\neq 1} \alpha_{1,j}\sigma_j + \left(\sum_{i<j, i\neq 1} \alpha_{ij} g_{ij} + \alpha_0 \right) = 0$$

Since $\sigma_1 \in \{-1, 1\}$, this means both sums on the left hand side are zero. That is,

$$\sum_{j\neq 1} \alpha_{1,j}\sigma_j = 0 \tag{4.2.1}$$

This implies, $\alpha_{1,j} = 0$ for all $j > 1$. Continuing this way, it follows that $\alpha_0, \alpha_{ij} = 0$ for all $1 \leq i < j \leq n$.

□

Now, the proof of the Theorem 4.1.2 follows through for the case of spin systems. This provides a

way to determine the measure that realizes the given spin-spin correlations. If we choose $\Psi \equiv 1$, we get the maximum entropy measure that realizes the given correlations.

Let's look at the Euler scheme for the above differential equation.

1. Set an initial value λ_1.
2. Set $r = 1$
3. Calculate $u(\lambda_r) = \sum \frac{1}{Z} G e^{-G^T \lambda_r}$
4. Update λ using
$$\lambda_{r+1} = \lambda_r - M(\lambda_r)^{-1}(R - u(\lambda_r))$$
5. Until $r = K$

The convergence of this Euler scheme to the "right" value of λ is not clear; moreover it involves the inversion of a matrix, which can be computationally hard in high dimension. In the next section, we consider a modification of the above scheme, for which we can prove convergence, and that does not involve matrix inversion. However, before going into the details, let us look at some general theory and important results for multi-dimensional, first-order, non-linear discrete dynamical systems.

4.2.1 Discrete Dynamical Systems

Consider a system of non-linear first order difference equations

$$x_{t+1} = \phi(x_t), \qquad t = 0, 1, 2, \ldots$$

where $\phi : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ and $x_0 = (x_0^1, x_0^2, \ldots . x_0^n)$ is given.

A solution to the difference equation $x_{t+1} = \phi(x_t)$ is a trajectory (or an orbit) of the vector $(x_t)_t^\infty$ that satisfies this law of motion at every point in time starting at x_0.

Definition 4.2.1. A steady state equilibrium or a fixed point of the system $x_{t+1} = \phi(x_t)$ is a vector $x^* \in \mathbb{R}^n$ such that
$$x^* = \phi(x^*)$$

A non-linear dynamical system is characterized by existence of a unique steady state equilibrium, existence of multiple steady state equilibria, or by non-existence of a steady state equilibrium. Moreover, a non-linear system may converge to a steady state equilibrium or to a periodic orbit or may diverge to $\pm\infty$. Unlike a linear system, non-linear system may exhibit chaotic behavior. The study of steady state of a non-linear system usually involves approximation of the system in the neighborhood of x^*. A steady state equilibrium x^* is called globally (asymptotically) stable if the system converges to this steady state independently of the initial condition. It is called locally (asymptotically) stable if there exists a small neighborhood of x^* such that for every initial condition within this neighborhood, the system converges to x^*. Formally,

Definition 4.2.2. A steady state equilibrium x^* of the system $x_{t+1} = \phi(x_t)$ is:

- Globally (asymptotically) stable, if

$$\lim_{t\to\infty} x_t = x^* \quad \text{for all } x_0 \in \mathbb{R}^n$$

- Locally (asymptotically) stable, if there exists $\varepsilon > 0$ such that $\lim_{t\to\infty} x_t = x^* \quad$ for all $x_0 \in B_\varepsilon(x^*)$

  where $B_\varepsilon(x^*) = \{x \in \mathbb{R}^n : |x_i - x_i^*| < \varepsilon \quad \forall\, i = 1, 2, \ldots, n\}$ is an $\varepsilon-$ball around x^*.

This means that if we perturb the system and if the system converges asymptotically to the original steady state regardless of the magnitude of the perturbation, then the system is globally stable. Whereas, if the system converges to the original steady state if we ensure that the perturbation is sufficiently small, then the system is only locally stable.

Remark 4.2.1. Global stability of a steady state equilibrium necessitates global uniqueness of the steady state equilibrium. Similarly, local stability of a steady state equilibrium necessitates local uniqueness of the steady state equilibrium.

We will now state the sufficient conditions for local and global stability of discrete systems but before that we introduce two more concepts.

Definition 4.2.3. Consider a map $\phi : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ and let $D\phi(x^*)$ be the Jacobian of ϕ evaluated at a steady state equilibrium x^*. The steady state equilibrium x^* is a hyperbolic fixed point if $D\phi(x^*)$ has no eigenvalues of modulus 1.

Definition 4.2.4. Let $(\mathcal{E}^n, d)$ be a metric space. Then, $\phi : \mathcal{E}^n \longrightarrow \mathcal{E}^n$ is a contraction mapping if for some $\rho \in (0, 1)$

$$d(\phi(x^1), \phi(x^2)) \leq \rho d(x^1, x^2) \qquad \forall\, x^1, x^2 \in \mathcal{E}^n$$

Sufficient conditions for Local stability

Theorem 4.2.1. *Let $\phi : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ be a $\mathcal{C}^1$ diffeomorphism with a hyperbolic fixed point x^*. The, the steady state equilibrium x^* is locally (asymptotically) stable if and only if the moduli of all the eigenvalues of $D\phi(x^*)$ are smaller than* 1.

Sufficient conditions for Global stability

Theorem 4.2.2. *A steady state equilibrium of a multi-dimensional, first order difference equation $x_{t+1} = \phi(x_t)$ exists, is unique and is globally stable if $\phi : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ is a contraction mapping.*

Having established the sufficient conditions for the local and global stability of a multi-dimensional, first order, non-linear discrete dynamical system, we can now proceed to discuss in detail our method for obtaining the probability measure that realizes the given spin covariances.

4.2.2 A new approach for Spins

We propose a new dynamical system in discrete time that converges to a λ which gives the measure that realizes the correlations.

Let us recall the the discussion on Maximum Entropy Problem for Spins in chapter 3, section 3.2.2. We consider the Dual functional obtained in (3.2.5):

$$\mathcal{J}(\lambda) = \sum_{h,k} \lambda_{hk} c_{hk} + \log \left[\sum_{\sigma \in S} \exp \left\{ - \sum_{h,k} \lambda_{hk} \sigma_h \sigma_k \right\} \right]$$

Note that, $\nabla \mathcal{J} = 0$ implies $\mathcal{P}^*(\sigma)$ satisfies the constraints. A critical point exists if $\mathcal{J}$ is proper, which means,

$$\lim_{|\lambda| \to \infty} \mathcal{J}(\lambda) = +\infty$$

We have seen that a rather large set of inequalities determine the set Δ_n (described in (3.2.6)). These inequalities ensure the properness of J and hence the feasibility of given correlations. In the following discussion, we assume that the feasibility of the correlations is known and we want to find a consistent measure.

We denote by R the vector of correlations

$$R = [c_{1,2}, \ldots, c_{1,n}, c_{2,3}, \ldots, c_{n-1,n}]$$

and,

$$\lambda = [\lambda_{1,2}, \ldots, \lambda_{1,n}, \lambda_{2,3}, \ldots, \lambda_{n-1,n}]$$
$$G = [g_{1,2}, \ldots, g_{1,n}, g_{2,3}, \ldots, g_{n-1,n}]$$

where $g_{ij} = \sigma_i \sigma_j$.

For convenience, we denote these random functions by $[X_1, X_2, \ldots, X_N]$, where $N = \frac{n(n-1)}{2}$.

With the above notation, we can write the dual functional as follows:

$$\mathcal{J}(\lambda) = R^T \lambda + \log \left[\sum_{\sigma \in S} e^{-G^T \lambda} \right]$$

where $G^T = G(\sigma)^T$. We omit the σ for notational convenience.

We want this function to have a global minimum, that is, we want

$$\nabla \mathcal{J}(\lambda) = R^T - \frac{\sum_{\sigma \in S} G^T e^{-G^T \lambda}}{\sum_{\sigma \in S} e^{-G^T \lambda}} = 0$$

The Hessian of $\mathcal{J}$ is given by,

$$H(\mathcal{J}(\lambda)) = \frac{\sum\limits_{\sigma\in S} G^T G e^{-G^T\lambda}}{\sum\limits_{\sigma\in S} e^{-G^T\lambda}} - \frac{\left(\sum\limits_{\sigma\in S} G e^{-G^T\lambda}\right)\left(\sum\limits_{\sigma\in S} G^T e^{-G^T\lambda}\right)}{\left(\sum\limits_{\sigma\in S} e^{-G^T\lambda}\right)^T}$$

Lemma 4.2.2. *$H(\mathcal{J}(\lambda))$ is strictly positive definite.*

Proof. Notice that under the probability $P(\sigma) = \frac{1}{Z}e^{-G^T\lambda}$,

$H(\mathcal{J}(\lambda)) = Var(G)$ where $Var(G)$ denotes the variance-covariance matrix of the vector G.

Then, it is clear that $H(\mathcal{J}(\lambda)) \geq 0$ (all variance-covariance matrices are positive semi-definite). If $Var(G)$ is not strictly positive definite, then there exists a not zero vector b such that $b^T Var(G) b = 0$. That is, $Var(bG) = 0$. This implies that bG is a constant with probability 1.

$$\sum b_i X_i = a$$

for some fixed constant a. This shows that to prove that $Var(G)$ is non-singular, it is enough to show that $X_i's$ (or $g_{ij}'s$) are linearly independent which follows from lemma 4.2.1. □

Thus, $H := H(\mathcal{J}(\lambda)) > 0$, which means that $\mathcal{J}(\lambda)$ is a strictly convex function with a global minimum at say $\tilde{\lambda}$ (where $\tilde{\lambda}$ is such that $\nabla\mathcal{J}(\tilde{\lambda}) = 0$).

Lemma 4.2.3. *The eigenvalues of the Hessian H are bounded by $n(n-1)/2$.*

Proof. We know that H is the variance-covariance matrix of random variables $X_1, X_2, \ldots, X_N$,where $N = n(n-1)/2$. Let O be an orthogonal matrix which diagonalizes H. Without loss of generality, we can assume that $\delta_1 = \sum O_{1,i} H_{i,j} O_{j,1}$ is the largest eigenvalue of H. Then,

$$\begin{aligned}
\delta_1 &= \sum O_{1,i} H_{i,j} O_{j,1} \\
&= \sum Cov(O_{1,i}X_i, O_{j,1}X_j) \\
&= Var(\sum O_{1,i}X_i) \\
&\leq E[\sum (O_{1,i}X_i)^2] \\
&\leq E[\sum (O_{1,i})^2 \sum (X_i)^2] \\
&\leq E[\sum (X_i)^2] \\
&\leq N
\end{aligned}$$

□

Let us consider the dynamics given by

$$\lambda_{n+1} = \lambda_n - \frac{1}{K}\nabla\mathcal{J}(\lambda)$$

where $K > N$.

To prove that this difference equation converges to a fixed point that is globally stable it is sufficient to prove the following:

Theorem 4.2.3. *The map*

$$\phi : \lambda \longmapsto \lambda - \frac{1}{K}\nabla\mathcal{J}(\lambda)$$

is a contraction for $K > N$.

Proof. To show that the above map is a contraction, we have to show that

$$\|\phi(\lambda_h) - \phi(\lambda_k)\| \leq \rho\|\lambda_h - \lambda_k\|$$

for some $\rho \in (0, 1)$.

Denote by f the function $\nabla\mathcal{J}$. Then,

$$\begin{aligned}\|\phi(\lambda_h) - \phi(\lambda_k)\| &= \|\lambda_h - \lambda_k + \frac{1}{K}(f(\lambda_k) - f(\lambda_h))\| \\ &= \|\lambda_h - \lambda_k - \frac{1}{K}H(\lambda')(\lambda_h - \lambda_k)\|\end{aligned}$$

where $H(\lambda')$ is Hessian of $\mathcal{J}$ at point λ', a point on the line joining λ_h and λ_k.

$$\|\phi(\lambda_h) - \phi(\lambda_k)\| = \|(I - \frac{1}{K}H(\lambda'))(\lambda_h - \lambda_k)\|$$

Or,

$$\|\phi(\lambda_h) - \phi(\lambda_k)\| \leq \|(I - \frac{1}{K}H(\lambda'))\|\|(\lambda_h - \lambda_k)\|$$

$\|(I - \frac{1}{K}H(\lambda'))\| =$ (maximum eigenvalue of $(I - \frac{1}{K}H(\lambda'))^2)^{1/2} = \max_{1\leq i\leq N}\left\{1 - \frac{1}{K}\delta_i\right\}$, where δ_i are eigenvalues of $H(\lambda')$. From lemma 4.2.3, we know that the eigenvalues of H are less or equal to N. This means,

If,

$$\rho = \|(I - \frac{1}{K}H(\lambda'))\|$$

Then,

$$0 < \rho < 1 \quad \text{and} \quad \|\phi(\lambda_h) - \phi(\lambda_k)\| \leq \rho \|\lambda_h - \lambda_k\|$$

Thus, ϕ is a contraction.

□

Thus, we now have a discrete time dynamical system given by

$$\lambda_{n+1} = \lambda_n - \frac{1}{K} \nabla \mathcal{J}(\lambda) \qquad \text{for } K > N$$

that converges to the right λ. The fact that it converges to a λ that is the unique globally stable steady state of this system follows from theorem 4.2.2.

This system can now be solved to obtain explicitly the required probability measure. Note that this does not test the feasibility of the given correlations. It gives the λ that parametrizes the maximum entropy measure. The crucial advantage of this method is that it is in discrete time and hence one can write stochastic algorithms to solve it approximately. We shall see in the next chapter that these stochastic algorithms are much faster for large n.

Chapter 5

Markov Chain monte Carlo

5.1 Monte Carlo Methods: Introduction

Monte Carlo methods are used in wide variety of problems. One of the most important uses of Monte Carlo methods is in evaluating multi-dimensional integrals which can be approximated in a much quicker time by Monte Carlo in comparison to other techniques. The basic idea is the following.

Suppose we are given a random variable X (that has finite moments) and we want to calculate the expected value as $A = \mathbb{E}[X]$. If we can generate $X_1, \ldots, X_n$, n independent random variables with the same distribution, we can make the approximation

$$A \approx \hat{A}_n = \frac{1}{n} \sum_{k=1}^{n} X_k$$

Then, by the strong law of large number we have $\hat{A}_n \to A$ a.s. as $n \to \infty$.

One can categorize Monte Carlo experiments into two broad classes: (1) Simulation of random systems and (2) Adding artificial randomness to a system and then simulating the new system. Monte Carlo is most commonly used as a tool for calculating multi-dimensional integrals. The first kind of problems usually involve simulation of a stochastic process and then approximating the mean or the higher moments. Whereas, in the second kind the system could be completely deterministic. We represent the problem as a different random system and then simulate this new system to approximate the behaviour of the original system. To understand these notions more clearly, we give some examples:

Example 10. ***Queueing***. *Consider a queueing system composed of a network of servers serving a stream of incoming streams like switches in a telecommunication network. Some of the key*

variables characterizing such a system are:

(a) the arrival time of the i-th customer at the various servers.

(b) the service time of the i-th customer.

(c) rules for customers proceeding from one server to another.

(d) characteristics of different classes of customers.

By simulating these random variables, one can simulate the queueing system.

Example 11. ***Estimating the value of*** π. *As we know, there are efficient deterministic algorithms to estimate the value of* π. *However, we can introduce randomness to the system and try and estimate it using Monte Carlo. Consider a circle of diameter* 2 *that lies inside a* 2×2 *square. Pick a point* A_1 *uniformly at random inside the square. The probability that the point lies in the circle is* $\pi/4$. *Repeat this* n *times. Then, we have* $A_1, A_2, \ldots, A_n$ *each uniformly (and independently) distributed inside the square. Let* Z *be the number of* A_i*'s that lie inside the circle. Then,* Z *is binomially distributed with parameters* n *and* $\pi/4$. *Thus, we have* $\mathbb{E}(Z) = n\pi/4$ *or* $\mathbb{E}(4Z/n) = \pi$. *We can fix* n *and then observe* Z, *say* m *times to estimate* π *by* $4m/n$.

Example 12. ***Finding the minimum or maximum of a function***. *Consider the problem of finding minimum (or maximum) of a deterministic function say* $\mathcal{H}(x)$ *on* $\mathbb{R}$. *Clearly, here there is no integral to calculate and the problem is completely deterministic. However, we can introduce randomness by considering a density function given by*

$$f(x) = \frac{1}{Z} e^{-\beta \mathcal{H}(x)}$$

where Z *is the normalization factor. Then, for* $\beta > 0$, *the global maximum of* f *approximates the global minimum of* $\mathcal{H}(x)$. *We are assuming that the problem is feasible, that is, the maximum (or minimum) does exist. The idea is to create a sequence of points* $X_1, X_2, \ldots$ *that are approximately distributed according to pdfs* $f_1(x), f_2(x), \ldots$ *with* $f_t(x) \sim f_{\beta_t}(x) = \frac{1}{Z} e^{-\beta_t \mathcal{H}(x)}$ *where* $\beta_t \to \infty$. *If each* X_t *were sampled exactly from* $f_{\beta_t}(x)$, *then* X_t *would converge to a global maximum of* $f(x)$ *as* $\beta_t \to \infty$.

There are three important parts of applying Monte Carlo Method to a particular system.

- **Generation.** This involves generating random numbers or vectors (as the case may be) that have a specified distributions. We will discuss this is a little more detail in the next section.
- **Accuracy.** How accurate can we expect our answer to be? For this we need to understand the behavior of the random process being simulated and study how rapidly the process converges to the solution.
- **Efficiency.** How efficient is our algorithm? This is essentially a question of algorithmic efficiency. We need to know how the Monte Carlo Method fares compared to other methods in terms of computer time needed to get to the solution. As indicated earlier, Monte Carlo is in general not ideal for low dimensional problems but is far better in high dimensions.

While the way to determine accuracy and efficiency largely depends on the problem, there is a general theory on sampling random numbers from a specified distribution. We discuss some of the well known methods for sampling in the next section.

5.2 Sampling techniques

In this section, we will look at various algorithms for sampling from given distributions.

5.2.1 Sampling from a Uniform Distribution

Most of the programing languages have functions to generate pseudo random numbers which are distributed according to the standard uniform distribution.

In general, a pseudo random generator is a deterministic recurrence relation

$$X_{t+1} = f(X_i, X_{i-1}, \ldots, X_{i-s}) \qquad (i \geq s)$$

for some fixed integer $s \geq 0$. The recursion requires an initial vector of random seeds $(X_s, X_{s-1}, \ldots, X_0) \in \mathbb{R}^{n+1}$ which must be supplied in the beginning. A simple algorithm for generating random number would be as follows:

1. Draw the seed S_0 from a distribution μ on the set of states S. Set $t = 1$.
2. Set $S_t = f(S_{t-1})$.
3. Set $X_t = g(S_t)$
4. Set $t = t + 1$, until $t = T$ for some T.

where, S is a finite set of states, f is a function from S to S, μ is a probability distribution on S, X is the output space and g is a function from S to X.
The algorithm produces a sequence $X_1, X_2, X_3, \ldots$ of pseudorandom numbers.

5.2.2 Sampling from a Non-Uniform Distribution

Although there are several methods for sampling, a lot of times they are specific to the target distribution. For example, the Box Muller method that generates two i.i.d. $N(0, 1)$ random variables from two i.i.d. $U[0, 1]$ random variables [23]. In this section, we look at some of the general methods to sample from a given distribution assuming we know how to sample from $U[0, 1]$.

Inversion method

Let F be a continuous cumulative distribution function, then for $y \in [0, 1]$, the generalized inverse distribution function F^{-1} if defined as:

$$F^{-1}(y) = \inf_{x \in \mathbb{R}} \{F(x) \geq y\}$$

The inversion method is very basic and is based on the following proposition

Proposition 5.2.1. *Let F be the cumulative distribution function of a random variable, and let U be a random variable such that $U \sim U[0,1]$. Then, $F^{-1}(U) \sim F$.*

Proof. Since F is right-continuous, for any $x \in \mathbb{R}$ we have

$$Pr\{F^{-1}(U) \leq x\} = Pr\{U \leq F(x)\} = F(x)$$

□

The inversion method involves generating a uniform random variable U and then setting $X = F^{-1}(U)$ to generate s random variable X with distribution given by F.

Rejection method

We want to generate a random variable X from a probability density function f. Suppose that f is bounded and supported on a closed interval $[a,b]$. Let $c = \sup\{f(x) : x \in [a,b]\}$. Then, the rejection method to generate $X \sim f$ is as follows:

1. Generate $Q \sim U[a,b]$ and $Y \sim U[0,c]$, where Q and Y are independent.
2. If $Y \leq f(Q)$, then accept and set $X = Q$. Stop.
   If $Y > f(Q)$, then reject and return to step 1.

This can be generalized to $n-$dimensional random vectors and to discrete setting.

Composition method

Give a probability density function f to sample from, we divide the region under the graph of f into a finite number of subregions, namely, $S_1, \ldots, S_M$ with respective areas $A_1, \ldots, A_M$ so that $\sum_{i=1}^{M} A_i = 1$. The, the composition method to generate $X \sim f$ is as follows:

1. Generate $I \in \{1, \ldots, M\}$ with probability mass function. $\{A_1, \ldots, A_M\}$.
2. Generate (V, W) uniformly on S_I (This means consider $S_I = X_I \times Y_I$, that is, cartesian product of two axes. Then, generate independent random variables U on X_I and V on Y_I).
3. Set X = V.

5.3 Markov Chain Monte Carlo (MCMC)

Before going into details of Markov Chain Monte Carlo Algorithms, let us establish some notation and known facts about Markov chains.

5.3.1 Markov Chains

We shall consider a discrete-time time homogenous Markov chain $X_0, X_1, X_2 \ldots$ where each X_i takes values in a finite or countable state space $\mathcal{S}$. The transition probability matrix is given by $P = ((p_{ij}))$ and the $k-$step probabilities are:

$$p_{ij}^k = Pr(X_{t+k} = j | X_t = i) \qquad\qquad i, j \in \mathcal{S}$$

With the above notation, p_{ij}^k is the (i, j)-th entry of P^k. The transition probabilities are independent of time because we are assuming time homogeneity of the Markov Chain. This is a reasonable assumption for many models. In context of Monte Carlo Markov Chain algorithms where one is looking for a Markov chain with a given stationary distribution, time homogeneity is rather natural.

A Markov chain is irreducible if the chain can eventually get from each state to every other state, that is, for every $i, j \in \mathcal{S}$, there exists a $k \leq 0$ (depending on i and j) such that $p_{ij}^k > 0$.

An irreducible chain has period T (where T is a positive integer) if T is the greatest common divisor of $\{k \geq 1 : p_{ii}^k > 0\}$ for some $i \in \mathcal{S}$ (equivalently, for all $i \in \mathcal{S}$).

A chain is called aperiodic if its period is 1. In particular, if an irreducible chain has $p_{ii} > 0$ for some i, then it is aperiodic.

Theorem 5.3.1. *Consider an aperiodic irreducible Markov chain with state space $\mathcal{S}$. For every $i, j \in \mathcal{S}$, the limit $\lim_{k\to\infty} p_{ij}^k$ exists and is independent of i. We call this limit π_j. Then*

- *If $\mathcal{S}$ finite, then*

$$\sum_{j\in\mathcal{S}} \pi_j = 1 \qquad \textit{and} \qquad \sum_{i\in\mathcal{S}} \pi_i p_{ij} = \pi_j$$

  for every $j \in \mathcal{S}$. In other words, if we write $\pi = ((\pi_i))$ as a row vector, then $\pi P = \pi$. Moreover the only solution of

$$\begin{cases} vP = v \\ \sum_i v = 1 \\ v_i \geq 0 \end{cases} \tag{5.3.1}$$

  is $v = \pi$.

- *If $\mathcal{S}$ is countably infinite, then either (a) $\pi_j = 0$ for every j in which case there is no solution of* (5.3.1) *or (b) π satisfies* (5.3.1) *and is the unique solution of* (5.3.1).

The chain is said to be positive recurrent in this case (except when $\pi_j = 0$ for every j) and π's are called the stationary or equilibrium distributions.

Proposition 5.3.1. *Consider an irreducible Markov chain with discrete state space $\mathcal{S}$ Assume that there exist positive numbers π_i for every $i \in \mathcal{S}$ such that $\sum_i \pi_i = 1$ and*

$$\pi_i p_{ij} = \pi_j p_{ji} \quad \textit{for every } i, j \in \mathcal{S}$$

Then, $\pi = (\pi_i)_{i \in \mathcal{S}}$ is the stationary distribution.

Proof. We have, $\pi_i p_{ij} = \pi_j p_{ji}$ for every $i, j \in \mathcal{S}$. Hence,

$$\sum_{i \in \mathcal{S}} \pi_i p_{ij} = \sum_{i \in \mathcal{S}} \pi_j p_{ji} = \pi_j \sum_{i \in \mathcal{S}} p_{ji} = \pi_j$$

which means $\pi P = \pi$.

□

Definition 5.3.1. If there exist positive numbers π_i such that $\pi_i p_{ij} = \pi_j p_{ji}$, then the chain is called reversible.

Indeed, for a chain X with stationary distribution π, we have

$$\begin{aligned} Pr(X_t = i, X_{t+1} = j) &= \pi_i p_{ij} p_{jk} \\ &= \pi_j p_{ji} \\ &= \pi_j p_{ji} \\ &= Pr(X_t = j, X_{t+1} = i) \end{aligned}$$

Definition 5.3.2. A Markov chain is called symmetric if $p_{ij} = p_{ji}$ for every i and j. In other words, a Markov chain is called symmetric if the corresponding transition probability matrix is symmetric.

Corollary 5.3.2. *Suppose that an irreducible Markov chain on the finite state space $\mathcal{S}$ is symmetric. Then the stationary distribution is uniform on $\mathcal{S}$, that is, $\pi_i = 1/|\mathcal{S}|$ for all $i \in \mathcal{S}$, where $|\mathcal{S}|$ denotes cardinality of $\mathcal{S}$.*

Theorem (4.1) is an important result in context of Markov Chain Monte Carlo simulation. It can be interpreted as follows:

- $\pi_i \approx P(X_t = i)$ for large t, is independent of the distribution of X_0.
- Over a large period of time, π_i is the fraction of time the system spends in the state i.
- In the positive recurrent case, π is the stationary distribution. This means that if $X_t \sim \pi$ then $X_s \sim \pi$ for every time $s > t$.

Suppose we are given a probability distribution f on a set $\mathcal{S}$ and we want to generate random elements of $\mathcal{S}$ with distribution. This problem can be solved using the sampling techniques discussed before but we can also use MCMC (Markov Chain Monte Carlo) for the same. The idea is to come up with an irreducible Markov chain whose equilibrium distribution is f and then simulating the chain for a long time. In the long run, the output of the chain should approximately follow the distribution f. Again, there are some known methods for constructing the chains. We will discuss two important methods for constructing chains for non-uniform distributions but before that let's understand the idea behind MCMC in more detail.

5.4 MCMC: Algorithms

We will state the problem is full generality here. The problem addressed by MCMC algorithms is the following. We are given a density function π, on a state space $\mathcal{S}$, which is possibly unnormalised but satisfies $0 < \sum_{\mathcal{S}} \pi(x) < \infty$.

This density gives rise to a probability measure $\pi(.)$ on $\mathcal{S}$, by

$$\pi(A) = \frac{\sum_A \pi(x)}{\sum_{\mathcal{S}} \pi(x)}$$

Suppose we want to estimate expectations of functions $f : \mathcal{S} \longrightarrow \mathbb{R}$ with respect to $\pi(.)$, i.e. we want to estimate

$$\pi(f) = \mathbb{E}_\pi[f(X)] = \frac{\sum_{\mathcal{S}} f(x)\pi(x)}{\sum_{\mathcal{S}} \pi(x)}$$

As we have learned before, the classical Monte Carlo solution to this problem is to simulate i.i.d. random variables $X_1, X_2, \ldots X_m \sim \pi(.)$, and then estimate $\pi(f)$ by

$$\hat{\pi}(f) = \frac{1}{m} \sum_{i=1}^{m} f(X_i)$$

However, if π is complicated, then it is very difficult to directly simulate i.i.d. random variables from $\pi(.)$.

The Markov chain Monte Carlo (MCMC) method provides an alternative way that is easier to run on a computer. The idea is to construct a Markov chain on $\mathcal{S}$ which has $\pi(.)$ as a stationary distribution. That is, we want to define easily-simulated Markov chain transition probabilities $P(x, y)$ for $x, y \in \mathcal{S}$, such that

$$\sum_{x \in \mathcal{S}} \pi(x)P(x, y) = \pi(y)$$

Then if we run the Markov chain (provided it satisfies certain conditions) for a long time (started

from anywhere), then for large n the distribution of X_n will be approximately stationary.

There are two very important methods that illustrate how to go about construction a Markov chain for application of MCMC. We look at thee methods now. Keeping in mind the context of this thesis, we present them and the corresponding proof for the discrete case.

5.4.1 The Metropolis Algorithm

Let $\mathcal{S}$ be a discrete state space (finite or countable). Let Q be a symmetric transition probability matrix. Let π be any probability distribution on $\mathcal{S}$ with $\pi_i > 0$ for all $i \in \mathcal{S}$. This π is our target distribution. That is, we want to sample from π.

We want to define a Markov chain $X = X_0, X_1, \ldots$ on $\mathcal{S}$. Given, $X_t = i$, then the next state X_{t+1} is determined by the Metropolis algorithm as follows:

1. Choose $Y \in \mathcal{S}$ randomly according to the Markov chain Q, that is

   $$Pr(Y = j | X_t = i) = q_{ij}$$

   for every $j \in \mathcal{S}$

2. Let $\alpha = \min\{1, \pi_Y/\pi_i\}$ (α is called the acceptance probability)

3. Accept Y with probability α. That is generate a random variable $U \sim U[0,1]$. If $U \leq \alpha$, then accept the proposal and set $X_{t+1} = Y$. If $U > \alpha$, then reject the proposal and set $X_{t+1} = X_t$.

This Markov chain has transition probabilities

$$p_{ij} = \begin{cases} q_{ij} \min\{1, \pi_j/\pi_i\} & \text{if } j \neq i \\ 1 - \sum_{k,k\neq i} q_{ik} \min\{1, \pi_k/\pi_i\} & \text{if } j = i \end{cases}$$

Proposition 5.4.1. *Assume that Q is an irreducible symmetric Markov chain on $\mathcal{S}$, and π is a strictly positive probability distribution on $\mathcal{S}$. Then the metropolis chain defined above is irreducible and reversible with respect to π.*

Proof. Irreducibility follows from the irreducibility of Q since $p_{ij} > 0$ whenever $q_{ij} > 0$. For reversibility, we need to check $\pi_i p_{ij} = \pi_j p_{ji}$ for every i and j. This is trivial for the case $i = j$. For $i \neq j$,

$$\pi_i p_{ij} = q_{ij}(\pi_i \min\{1, \pi_j/\pi_i\}) = q_{ij} \min\{\pi_i, \pi_j\}$$

which is symmetric in i and j since Q is symmetric.

□

5.4.2 The Gibbs Sampler

Let π be a discrete probability distribution on $\mathcal{S} \subset \mathbb{R}^n$ and let V be a random vector with distribution π. For every $j = 1, 2, \ldots, n$ define the matrix P_j by

$$\begin{aligned} P_j(z, w) &= Pr\{V = w | V_{-j} = z_{-j}\} \\ &= \begin{cases} 0 & \text{if } w_{-j} \neq z_{-j} \\ \pi(w)/\pi_{-j}(z_{-j}) & \text{if } w_{-j} = z_{-j} \end{cases} \end{aligned}$$

where, $\pi_{-j}(z_{-j}) = Pr\{V_{-j} = z_{-j}\}$

Now, define

$$P_{RS} = \frac{1}{m} \sum_{j=1}^{n} P_j$$

This is the transition matrix for the random scan Gibbs sampler. Next, we define

$$P_{SS} = P_1 P_2 \ldots P_m$$

this is the transition matrix of the systematic scan Gibbs sampler.

Proposition 5.4.2. *For the above definitions:*

- *Each of $P_1, P_2, \ldots, P_m$ and P_{RS} is reversible with respect to π.*
- *π is a stationary distribution for P_{SS}, even though P_{SS} need not be reversible.*

Proof. For the first part, fix $k \in \{1, \ldots, m\}$. We need to show

$$\pi(z) P_k(z, w) = \pi(w) P_k(w, z) \quad \text{for all } z, w \in \mathcal{S} \tag{5.4.1}$$

If $z_{-k} \neq w_{-k}$, then $P_k(w, z) = 0 = P_k(z, w)$ and so (2) holds trivially in this case. Now, if $z_{-k} = w_{-k}$, then

$$\pi(z) P_k(z, w) = \pi(z) \frac{\pi(w)}{\pi_{-k}(z_{-k})} = \frac{\pi(z)\pi(w)}{\pi_{-k}(w_{-k})} = \pi(w) P_k(w, z)$$

Therefore, each P_k is reversible. Now we will how that P_{RS} is reversible.

$$\begin{aligned}\pi(z)P_{RS}(z,w) &= \frac{1}{m}\sum_{k=1}^{m}\pi(z)P_k(z,w)\\ &= \frac{1}{m}\sum_{k=1}^{m}\pi(w)P_k(w,z)\\ &= \pi(w)P_{RS}(w,z)\end{aligned}$$

This completes the proof of first part. From the above and from proposition (4.1) we have $\pi P_k = \pi$ for each k. Therefore,

$$\pi P_{SS} = (\pi P_1)P_2 \dots P_m = (\pi P_2)P_3 \dots P_m = \dots = \pi$$

which completes the proof.

□

5.4.3 An important example: Ising Model

Let G be a graph with vertices V and set of edges E. We write $\langle i, j\rangle$ to denote the edge with endpoints of the vertices i and j and σ_i for the spin at vertex i. The vector $\sigma = (\sigma_1, \dots, \sigma_{|V|})$ denotes the vector of all spins. The Ising model is the probability distribution π^β on Ω_V(depending on a parameter $\beta \in \mathbb{R}$) that is defined as follows. Let

$$H(\sigma) = \sum_{\langle i,j\rangle \in E} \mathbb{1}_{[\sigma_i \neq \sigma_j]}$$

where $\mathbb{1}$ denotes the indicator function. Now, define

$$\pi^\beta(\sigma) = \frac{1}{C_\beta}\exp[-\beta H(\sigma)]$$

where

$$C_\beta = \sum_{\sigma \in \Omega_V} \exp[-\beta H(\sigma)]$$

is the normalizing constant. The function $H(\sigma)$ is called the Hamiltonian and it represents the energy of the configuration σ. Define the mean spin of σ by

$$M(\sigma) = \frac{1}{|V|}\sum_{i \in V}\sigma_i$$

It is hard to do exact calculations for the Ising model since a model with n spins has 2^n states. We can use MCMC to generate a sample $X_1, X_2, \ldots$ from π^β (for a given β).

We will now look at application of Metropolis Algorithm and Gibbs Sampler for the Ising model.

Metropolis algorithm

It is rather easy to adapt the Metropolis algorithm to the Ising model. For our proposal matrix Q, we use the simple random walk on $\{-1, 1\}^{|V|}$. Then, given $X_t = \sigma$

1. Pick $J \in V$ uniformly at random.
2. Set $Y = (\sigma_1, \ldots, \sigma_{J-1}, -\sigma_J, \sigma_{J+1}, \ldots, \sigma_{|V|})$. In other words, flip the J-th spin.
3. Let $\alpha = \min\left\{1, \frac{\exp[-\beta H(Y)]}{\exp[-\beta H(\sigma)]}\right\}$. Generate $U \sim U[0,1]$. If $U \leq \alpha$, then set $X_{t+1} = Y$. Otherwise set $X_{t+1} = \sigma$.

Gibbs sampler

To describe the transition matrices $P_k (k = 1, \ldots, |V|)$ for the Gibbs sampler, we introduce the following notation. For $\sigma \in \mathcal{S}$ and $k \in V$, let

$$\sigma^k[+] = (\sigma_1, \ldots, \sigma_{k-1}, 1, \sigma_{k+1}, \ldots, \sigma_{|V|})$$
$$\sigma^k[-] = (\sigma_1, \ldots, \sigma_{k-1}, -1, \sigma_{k+1}, \ldots, \sigma_{|V|})$$

Then,

$$\begin{aligned} P_k(\sigma, \sigma^k[+]) &= \frac{\exp\{-\beta H(\sigma^k[+])\}}{\exp\{-\beta H(\sigma^k[+])\} + \exp\{-\beta H(\sigma^k[-])\}} \\ &= \frac{1}{1 + \exp\{\beta(H(\sigma^k[+]) - H(\sigma^k[-]))\}} \end{aligned}$$

Write

$$H(\sigma^k[+]) = \sum_{\langle i,j\rangle : i \neq k, j \neq k} \mathbb{1}_{[\sigma_i \neq \sigma_j]} + \sum_{i : \langle i,k\rangle \in E} \mathbb{1}_{[\sigma_i \neq +1]}$$
$$H(\sigma^k[-]) = \sum_{\langle i,j\rangle : i \neq k, j \neq k} \mathbb{1}_{[\sigma_i \neq \sigma_j]} + \sum_{i : \langle i,k\rangle \in E} \mathbb{1}_{[\sigma_i \neq -1]}$$

Then we have,

$$H(\sigma^k[+]) - H(\sigma^k[-]) = \sum_{ik} \mathbb{1}_{[\sigma_i \neq +1]} - \mathbb{1}_{[\sigma_i \neq -1]}$$
$$= deg^-(k) - deg^+(k)$$

where $deg^-(k)$ (respectively $deg^+(k)$) is the number of neighbours i of vertex k such that σ_i equals -1 (respectively $+1$). We conclude that,

$$P_k(\sigma, \sigma^k[+]) = \frac{1}{1 + \exp\{\beta(deg^-(k) - deg^+(k))\}}$$
$$P_k(\sigma, \sigma^k[-]) = 1 - P_k(\sigma, \sigma^k[+])$$

5.5 MCMC: Convergence

It is evident that for any of the above algorithms to work, it is necessary for the constructed Markov chain to converge to its stationary distribution. We will discuss this issue is a fairly general setting in this section. We do not assume that the state space $\mathcal{S}$ is finite or countable. However, since most of the results follow trivially when the state space is finite, we state them without proofs. Before going into the important results, we define some key concepts. The proofs of the theorems and a more detailed discussion can be found in [29].

There are several ways of studying the stability of a Markov chain. One of the very first concepts is that of ϕ-irreducibility. The idea behind considering ϕ-irreducible chains is that for stability concerns it is desirable that the chain does not in reality consist of two chains. That is, the collection of sets which we can reach from different starting points is not different. This leads us to the definition of ϕ-irreducibility.

Definition 5.5.1. A chain is ϕ-irreducible if there exists a non-zero σ-finite measure ϕ on $\mathcal{S}$ such that for all $A \subseteq \mathcal{S}$ with $\phi(A) > 0$,and for all $x \in \mathcal{S}$, there exists a positive integer $n = n(x, A)$ such that $P^n(x, A) > 0$.

In other words, ϕ-irreducibility requires existence of a non-zero σ-finite measure ϕ on $\mathcal{S}$ such that for every starting point $x \in \mathcal{S}$ and for $A \subseteq \mathcal{S}$

$$\phi(A) > 0 \Longrightarrow P_x(\tau_A < \infty) > 0$$

where P_x denotes the probability of events conditional on the chain beginning with $X_0 = x$, τ denotes the hitting time from a point to a set, that is, $\tau_A = \inf\{n \geq 1 : X_n \in A\}$

Remark 5.5.1. For a finite or countable space chain ϕ-irreducibility is just the concept of irreducibility defined before, with ϕ taken as counting measure.

The next plausible requirement should be that of recurrence. There should be a possibility of reaching likely states from unlikely starting points, but that reaching such sets of states should

be eventually guaranteed. We have seen the definition of "positively recurrent" in the context of theorem (3.1). Here, we state the definition is complete generality

Definition 5.5.2. A chain is called recurrent if there is a measure μ guaranteeing that for every starting point $x \in \mathcal{S}$

$$\mu(A) > 0 \Longrightarrow P_x(\tau_A < \infty) = 1$$

and then, as a further strengthening, that for every starting point $x \in \mathcal{S}$

$$\mu(A) > 0 \Longrightarrow E_x[\tau_A] < \infty$$

for any $A \subseteq \mathcal{S}$.

Now we state the main asymptotic convergence theorem. This theorem assumes that the state space's σ-algebra is countably generated, but this is a very weak assumption which is true for e.g. any countable state space, or any subset of $\mathbb{R}^d$ with the usual Borel σ-algebra.

Theorem 5.5.1. *If a Markov chain on a state space with countably generated σ- algebra is ϕ-irreducible and aperiodic, and has a stationary distribution π, then for π-a.e. $x \in \mathcal{S}$,*

$$\lim_{n\to\infty} \|P^n(x,.) - \pi(.)\| = 0$$

In particular, $\lim_{n\to\infty} P^n(x, A) = \pi(A)$ *for all measurable $A \subseteq \mathcal{S}$.*

Th above theorem requires that the chain be ϕ-irreducible and aperiodic, and have stationary distribution π. The MCMC algorithms are created precisely so that $\pi(.)$ is stationary, so this requirement is not a problem. Furthermore,it is usually easy to verify that chain is ϕ-irreducible. Note that as mentioned earlier ϕ-irreducibility is a given when the state space is countable. Also, the aperiodicity almost always holds. So, the above theorem is really useful for MCMC algorithms.

Remark 5.5.2. In the particular case of spin systems, the state space Ω_n is in fact finite so ϕ-irreducibility is not really a concern for the case we will discuss later on.

5.5.1 Ergodicity

Definition 5.5.3. A state i is said to be ergodic if it is aperiodic and positive recurrent. If all states in an irreducible Markov chain are ergodic, then the chain is said to be ergodic.

Ergodicity basically means that there is an invariant regime described by a measure π such that if the chain starts in this regime (that is, if ϕ_0 has distribution π) then it remains in the regime, and moreover if the chain starts in some other regime then it converges in a strong probabilistic sense with π as a limiting distribution.

Theorem (6.1) implies asymptotic convergence to stationarity, but it does not say anything about the rate of this convergence. One qualitative convergence rate property is uniform ergodicity:

Definition 5.5.4. A Markov chain having stationary distribution π is uniformly ergodic if

$$\|P^n(x,.) - \pi(.)\| \leq M\rho^n \qquad n = 1, 2, 3, \ldots$$

for some $\rho < 1$ and $M < \infty$.

One equivalence of uniform ergodicity is:

Theorem 5.5.2. *A Markov chain with stationary distribution π is uniformly ergodic if and only if $\sup_{x\in\mathcal{S}} \|P^n(x,.) - \pi(.)\| < 1/2$ for some $n \in \mathbb{N}$.*

A weaker condition than uniform ergodicity is geometric ergodicity.

Definition 5.5.5. A Markov chain having stationary distribution π is geometrically ergodic if

$$\|P^n(x,.) - \pi(.)\| \leq M\rho^n \qquad n = 1, 2, 3, \ldots$$

for some $\rho < 1$ and $M(x) < \infty$ for π-a.e. $x \in \mathcal{S}$.

The difference is that now the constant M may depend on the initial state x.

Definition 5.5.6. A subset $C \subseteq \mathcal{S}$ is small (or, (n_0, ϵ, ν)-small) if there exists a positive integer $n_0, \epsilon > 0$, and a probability measure ν on $\mathcal{S}$ such that the following *minorisation condition* holds:

$$P^{n_0}(x,.) \geq \epsilon\nu(.) \quad x \in C$$

That is, $P^{n_0}(x,.) \geq \epsilon\nu(A)$ for all $x \in C$ and all measurable sets $A \subseteq \mathcal{S}$.

This condition means that all of the n_0 - step transitions from within C, all have an "ϵ-overlap".

Definition 5.5.7. A Markov chain satisfies a drift condition (or, univariate geometric drift condition) if there are constants $0 < \gamma < 1$ and $b < \infty$, and a function $V : \mathcal{S} \to [1, \infty]$, such that

$$PV \leq \gamma V + b\mathbb{1}_C$$

That is, such that $\int_{\mathcal{S}} P(x, dy)V(y) \leq \gamma V(x) + b\mathbb{1}_C(x)$ for all $x \in \mathcal{S}$.

Then, we have the following theorem guaranteeing geometric ergodicity

Theorem 5.5.3. *Consider a ϕ-irreducible, aperiodic Markov chain with stationary distribution π. Suppose the minorisation condition is satisfied for some $C \subset \mathcal{S}$ and $\epsilon > 0$ and probability measure $\nu(.)$. Suppose further that the drift condition as defined above, is satisfied for some constants $0 < \gamma < 1$ and $b < \infty$, and a function $V : \mathcal{S} \to [1, \infty]$ with $V(x) < \infty$ for at least one (and hence for π-a.e.) $x \in \mathcal{S}$. Then the chain is geometrically ergodic.*

Of course, if the state space $\mathcal{S}$ is finite, then all irreducible and aperiodic Markov chains are geometrically (in fact, uniformly) ergodic. However, for infinite $\mathcal{S}$ this is not the case.

We now state an important theorem that throws some light on connections between various kind of stability ideas introduced in this section.

Theorem 5.5.4. *[25] The following four conditions are equivalent:*

1. *The chain admits a unique probability measure π satisfying the invariant equations*

$$\pi(A) = \int \pi(dx)P(x, A), \quad A \subseteq \mathcal{S}$$

2. *There exists some small set $C \subseteq \mathcal{S}$ and $M_C < \infty$ such that*

$$\sup_{x \in \mathcal{S}} E_x[\tau_C] \leq M_C$$

3. *There exists some small set C, some $b < \infty$ and some non-negative function V , finite ϕ-almost everywhere, satisfying*

$$P(x, dy)V(y) \leq V(x) - 1 + b\mathbb{1}_C(x), \quad x \in \mathcal{S}$$

4. *There exists some small set $C \subseteq \mathcal{S}$ and some $P^\infty(C) > 0$ such that*

$$\lim_{n\to\infty} \inf \sup_{x \in C} \|P^n(x, C) - P^\infty(C)\| = 0$$

Any of these conditions implies that for aperiodic chains,

$$\sup_{A \subseteq \mathcal{S}} \|P^n(x, A) - \pi(A)\| \to 0, \quad n \to \infty$$

for every $x \in \mathcal{S}$ for which $V(x) < \infty$, where V is any function satisfying (3).

5.6 MCMC for Spin Systems

Coming back to the problem of finding a probability measure that realizes given spin correlations, we have seen in chapter III that the discrete time dynamical system given by

$$\lambda_{n+1} = \lambda_n - \frac{1}{K}\nabla\mathcal{J}(\lambda) \qquad \text{for } K > N$$

converges to the right λ^* and by theorem 4.2.2, it follows that this λ^* is the unique globally stable steady state if the system.

We will now look at algorithms for solving this system. Suppose we are given λ_1 and we want to find λ that realizes the given vector of correlations R. λ_1 is just a starting point and can be initialized to something like $(1, 0, \ldots, 0)$.

Following the notation of chapter III, by $G(\sigma)$, we denote the column vector

$$(1, \sigma_1\sigma_2, \ldots, \sigma_1\sigma_n, \sigma_2\sigma_3, \ldots, \sigma_{n-1}\sigma_n)^T$$

of length $N = 1 + \frac{n(n-1)}{2}$ and by G^T we denote the transpose of G. Z denotes the normalizing constant given by $\sum_{\sigma\in\Omega} \exp(-G(\sigma)'\lambda)$. In everything that follows, $K = N + 1$.

We will first look at the deterministic algorithm.

Deterministic algorithm

1. Set an initial value λ_1.
2. Set $r = 1$
3. Calculate $u(\lambda_r) = \sum_\sigma \frac{1}{Z} G e^{-G^T\lambda_r}$
4. Update λ using
$$\lambda_{r+1} = \lambda_r - (R - u(\lambda_r))/K$$
5. $r = H$

Notice that in the above algorithm we must calculate $u(\lambda_r) = \sum_\sigma \frac{1}{Z} G e^{-G^T\lambda_r}$ and the normalizing factor Z. This involves calculating exponentials 2^n times in each loop. So, for large n this algorithm is rather slow. To overcome this problem of heavy calculations for large n, we propose a Markov Chain Monte Carlo algorithm.

MCMC algorithm

We have already seen the metropolis algorithm for the Ising model. We consider a Markov chain $\sigma^{(t)}$ with stationary distribution $\mu_\lambda = \frac{1}{Z} e^{-(G(\sigma^{(t)}))^T\lambda}$. Note that we update the parameter λ after every run of the Markov chain. The transition step of the chain involves flipping the k'th spin in the vector $\sigma^{(t)}$. Let us denote the new vector (after the flip) by $\tilde{\sigma}^{(t)}$. The transition probability is then given by:

$$\tilde{P}(\lambda_r) = \frac{e^{-(G(\sigma^{(t)}))^T\lambda_{r-1}}}{e^{-(G(\tilde{\sigma}^{(t)}))^T\lambda_{r-1}}}$$

The Markov chain is run for a time T for some T large enough to ensure the approximate convergence and then the parameter λ is updated in accordance with the theorem 4.2.3. This process is continued H times for some large enough H. The algorithm is as follows:

1. Set an initial value λ_1.
2. Set $r = 1$
3. Set $u = 0$, where u is a vector of order N.
4. Set initial value, $\sigma^{(0)}$, a starting point for the Markov chain.

5. Set $t = 1$ *Starting point of the Markov Chain*
6. Choose a random number between 1 to n and denote it by m.
7. Do $\sigma \longrightarrow \tilde{\sigma}$, by flipping the m^{th} spin.
8. Calculate the probability $\tilde{P}(\lambda_r)$ of the flip
9. Draw $h \sim$ Uniform$(0, 1)$
10. If $h \leq \tilde{P}(\lambda_r)$, accept the proposal and set $\sigma^{(t)} = (\tilde{\sigma})$
11. Calculate

$$u = u + G(\sigma^{(t)})/T$$

12. until $t = T$ *End of the Markov Chain*
13. Update λ using

$$\lambda_{r+1} = \lambda_r - (R - u(\lambda_r))/K$$

14. Until $r = H$.

We now look at a modification of above algorithm.

MCMC algorithm: with geometric update

Taking the idea of retaining the memory while we do the MCMC, we also test the following algorithm in the examples.

1. Set an initial value λ_1.
2. Set initial value, $\sigma^{(0)}$, a starting point for the Markov chain, $u = 0$ where u is a vector of order N and $0 < a < 1$.
3. Set $t = 1$
4. Set $w = 0$, where w is a vector of order N.
5. Set $s = 1$
6. Choose a random number between 1 to n and denote it by m.
7. Do $\sigma \longrightarrow \tilde{\sigma}$, by flipping the m^{th} spin.
8. Calculate the probability $\tilde{P}(\lambda_t)$ of flip
9. Draw $h \sim$ Uniform$(0, 1)$

10. If $h \leq \tilde{P}(\lambda_t)$, accept the proposal and set $\sigma^{(t)} = (\tilde{\sigma})$
11. Calculate

$$w = w + G(\sigma^{(t)})/S$$

12. until $s = S$
13. Set $u = u * a + w * (1 - a)$
14. Update λ using

$$\lambda_{t+1} = \lambda_t - (R - u^s(\lambda_t))/K$$

15. until $t = T$

The idea is the same as MCMC except for the fact that here we assign weight a to the older sample covariances to keep the memory.

We will now propose an algorithm for solving the same problem which updates λ and u simultaneously. This belongs to the class of algorithm that have come to be known as Adaptive Markov Chain Monte Carlo (Adaptive MCMC).

5.6.1 Adaptive Markov Chain Monte Carlo Methods

Again we describe the method in complete generality. Consider a probability space (Ω, A, P). We let $\{P_\theta : \theta \in \Theta\}$ be a parametric family of Markov kernels on (X, X). We consider a process $\{(X_n, \theta_n), n \geq 0\}$ and a filtration $\mathcal{F} = \{F_n, n \geq 0\}$ such that $\{(X_n, \theta_n), n \geq 0\}$ is adapted to $\mathcal{F}$ and for each n, and any non-negative function f,

$$\mathbb{E}[f(X_{n+1})|F_n] = P_{\theta_n} f(X_n) = \int P_{\theta_n}(X_n, dy) f(y), \quad P - \text{a.s.}$$

Let us look at the Adaptive MCMC for the problem of order n, in case of spin correlations.

Internal adaptive MCMC

The internal adaptive MCMC algorithm corresponds to the case where the parameter θ_n depends on the whole history $X_0, \ldots, X_n, \theta_0, \ldots, \theta_{n-1}$. However, it is often the case that the pair process $\{(X_n, \theta_n), n \geq 0\}$ is Markovian. The so-called controlled MCMC algorithm is a specific class of internal adaptive algorithms. According to this scheme, the parameter $\{\theta_k\}$ is updated according to a single step of a stochastic approximation procedure,

$$\theta_{k+1} = \theta_k + \gamma_{k+1} H(\theta_k, X_k, X_{k+1}), k \geq 0$$

where X_{k+1} is sampled from $P_{\theta_k}(X_k, .)$. In most cases, the function H is chosen so that the adaptation is easy to implement.

External adaptive MCMC

The external adaptive MCMC algorithms correspond to the case where the parameter process $\{\theta_n, n \geq 0\}$ is computed using an auxiliary process $\{Y_k, k \geq 0\}$ run independently from the process $\{X_k, k \geq 0\}$ (several auxiliary processes can be used as well). More precisely, it is assumed that the process is adapted to the natural filtration of the process $\{Y_k, k \geq 0\}$. That is, for each n, θ_n is a function of the history $(Y_0, Y_1, \ldots, Y_n)$ of the auxiliary process. In addition, conditionally to the auxiliary process $\{Y_k, k \geq 0\}$, $\{X_k, k \geq 0\}$ is an inhomogeneous Markov Chain, for any $0 \leq k \leq n$, and any bounded function f,

$$E[f(X_{k+1})|X_0, X_1, \ldots, X_k, Y_0, Y_1, \ldots, Y_k] = P_{\theta_k} f(X_k).$$

Note that in case of adaptive MCMC, the convergence of the parameter θ_k is not the central issue. The focus is on the way the simulations $\{X_k, k \geq 0\}$ approximate the stationary distribution π. The minimal requirements are that, the marginal distribution of X_k converges in an appropriate sense to the stationary distribution π, and that the sample mean $\frac{1}{n}\sum_{k=1}^{n} f(X_k)$, for the chosen f converges to $\pi(f)$. Some discussion on convergence in adaptive MCMC setting can be found in [2], [22].

5.6.2 Adaptive MCMC for the spin covariance realization problem

The idea of this algorithm is to build a Markov chain, similar to the one constructed above, but in which the parameter λ is updated at each step. Thus we obtain a single, non- homogeneous Markov chain that is expected to return the "right" λ in the limit of infinitely many iterations.

Adaptive MCMC algorithm

1. Set an initial value λ_1.
2. Set initial value, $\sigma^{(0)}$, a starting point for the Markov chain.
3. Set $t = 1$
4. Choose a random number between 1 to n and denote it by m.
5. Do $\sigma \longrightarrow \tilde{\sigma}$, by flipping the m^{th} spin.
6. Calculate the probability $\tilde{P}(\lambda_t)$ of flip
7. Draw $h \sim \text{Uniform}(0, 1)$

8. If $h \leq \tilde{P}(\lambda_t)$, accept the proposal and set $\sigma^{(t)} = (\tilde{\sigma})$
9. Calculate

$$u = \frac{(t-1)u + G(\sigma^{(t)})}{t}$$

10. Update λ using

$$\lambda_{t+1} = \lambda_t - (R - u(\lambda_t))/K$$

11. until $t = T$

Simulations show that the adaptive algorithm takes a long time to converge.

In the context of above discussion on adaptive MCMC, one can consider a modified version where instead of adapting the parameter θ_k at each step, it is adapted in batches, which can be computationally less demanding. With this in mind, we look at the following modifications of the adaptive algorithm.

Adaptive MCMC algorithm: Modification I

In the first modification of the above algorithm, we do the following: Instead of adapting λ_r continuously, we adapt it in batches of size T_0. This looks very similar to the original MCMC algorithm but we do not take T_0 to be very large which means we do wait for the convergence of the Markov chain and update the λ rapidly with the Markov chain, albeit in small intervals. More importantly, the sample mean u is not set to zero after each batch of T_0. This is a significant difference because this means that we completely retain the past information.

1. Set an initial value λ_1.
2. Fix T_0, the batch size over which λ is adapted.
3. Set initial value, $\sigma^{(0)}$, a starting point for the Markov chain.
4. Set $t = 1$
5. Choose a random number between 1 to n and denote it by m.
6. Do $\sigma \longrightarrow \tilde{\sigma}$, by flipping the m^{th} spin.
7. Calculate the probability $\tilde{P}(\lambda_t)$ of flip
8. Draw $h \sim \text{Uniform}(0, 1)$
9. If $h \leq \tilde{P}(\lambda_t)$, accept the proposal and set $\sigma^{(t)} = (\tilde{\sigma})$

10. Calculate

$$u = \frac{(t-1)u + G(\sigma^{(t)})}{t}$$

11. If $mod(t, T_0) = 0$, update λ using

$$\lambda_{t+1} = \lambda_t - (R - u(\lambda_t))/K$$

12. until $t = T$

Adaptive MCMC algorithm: Modification II

The second modification of the adaptive MCMC algorithm can be explained as follows:

Here, we keep the past information stored in a vector w and keep adding the new sample covariance $G(\sigma^{(t)})$ to it with each batch of size S of Markov chain. Thus, the covariance is calculated over $t * S$ samples at each step t. At each step t, we give a weight a to sample covariances calculated at $t - 1^{th}$ step.

1. Set an initial value λ_1, a such $0 < a < 1$.
2. Set initial value, $\sigma^{(0)}$, a starting point for the Markov chain.
3. Set $t = 1$
4. Set $w = 0$, where w is a vector of order N.
5. Set $s = 1$
6. Choose a random number between 1 to n and denote it by m.
7. Do $\sigma \longrightarrow \tilde{\sigma}$, by flipping the m^{th} spin.
8. Calculate the probability $\tilde{P}(\lambda_t)$ of flip
9. Draw $h \sim$ Uniform$(0, 1)$
10. If $h \leq \tilde{P}(\lambda_t)$, accept the proposal and set $\sigma^{(t)} = (\tilde{\sigma})$
11. Calculate

$$w = w + \frac{(t-1) * S * u^{t-1} + (1-a) * G(\sigma^{(t)})}{(t * S)}$$

12. until $s = S$
13. Set $u^t = a * w$

14. Update λ using

$$\lambda_{t+1} = \lambda_t - (R - u^t(\lambda_t))/K$$

15. until $t = T$

5.7 Some Examples

We implement the algorithms described in the previous sections in MATLAB to analyze and compare the results. We consider some of these examples here.

We consider the performance of each algorithm for small and large n. To look at the convergence of λ, we look at the plot of second entry of λ (which has been initialized to 0.5) with time (each iteration step is one time unit). We denote by R, the given matrix of covariances. We do not know whether it is realizable or not a priori, so, it is just a matrix in $M_n(\mathbb{R})$. We call it the matrix of covariances because if it is realizable then we try to find a measure μ_λ such that it realizes R as a covariance matrix of a spin system. The algorithms return a final λ. We use this parameter λ to construct the measure μ_λ and then calculate the R^* which is the corresponding covariance matrix. We want the algorithms to work well enough so that $R \approx R^*$ with a small error margin.

Before going into comparisons of various algorithms described in the previous section for a realizable matrix R, let us look at what happens if R is not realizable.

Example 13. *Consider a matrix*

$$R = \begin{pmatrix} 1 & 7 & 2 & 3 \\ 7 & 1 & 4 & 1 \\ 2 & 4 & 1 & 5 \\ 3 & 1 & 5 & 1 \end{pmatrix}$$

Clearly $R \notin \mathrm{Cov}_4$. As we have already seen in theorem 4.1.2, in the continuous time differential equation λ diverges while $M(\lambda)$ converges to a singular matrix. When the Euler scheme is used to approximate a solution, we observe a similar behaviour. In case of the discrete time deterministic algorithm, λ diverges and $R(\lambda)$ converges to the "nearest" boundary point. We get

$$R^* = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}$$

Below we consider an example where the Euler scheme doesn't work.

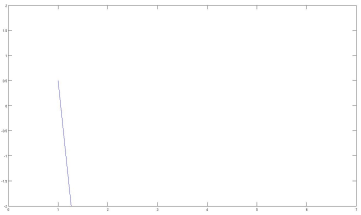

FIGURE 5.7.1: n = 4, Euler scheme for non feasible R

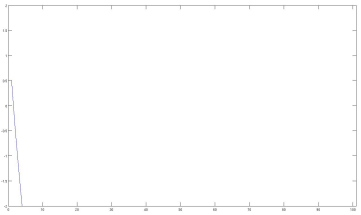

FIGURE 5.7.2: n = 4, Discrete deterministic algorithm for non feasible R

Example 14. *Let us consider*

$$A = \begin{pmatrix} 1 & 0.1 & 0.2 \\ 0.1 & 1 & 0.1 \\ 0.2 & 0.1 & 1 \end{pmatrix}$$

This is clearly a 3×3 *realizable spin correlation matrix. For* $n = 6$*, consider the block matrix*

$$R = \left(\begin{array}{c|c} A & A \\ \hline A & A \end{array}\right)$$

This is also realizable. However, we run into difficulties when we try to find a suitable λ *by finding an approximate solution to the differential equation using the Euler's method. This is because the matrix* $M(\lambda)$ *tends to be very close to a singular matrix. However, the same problem can be solved by using the deterministic algorithm. Since* R *is realizable, we know that the dual problem is feasible and that a fixed point of the contraction map* ϕ *as defined in section 4.2.2 of Chapter 4 exists. The deterministic algorithm then gives:*

$$\lambda = \begin{pmatrix} 1.0000 & 0.0419 & -0.0489 & -4.6742 & -0.0839 & -0.0489 \\ 0.0419 & 1.0000 & -0.0211 & -0.0839 & -4.6819 & -0.0211 \\ -0.0489 & -0.0211 & 1.0000 & -0.0489 & -0.0210 & -4.6741 \\ -4.6742 & -0.0839 & -0.0489 & 1.0000 & 0.0418 & -0.0489 \\ -0.0839 & -4.6819 & -0.0210 & -0.0418 & 1.0000 & -0.0210 \\ -0.0489 & -0.0211 & -4.6741 & -0.0489 & -0.0210 & 1.0000 \end{pmatrix}$$

for which the R *is realized.*

Thus, the deterministic algorithm has a clear advantage over finding an approximate solution of the differential equation because many a times when the matrix M is close to being singular, the Euler scheme becomes fragile. The deterministic algorithm, on the other hand, works in all cases. Let us start now compare the deterministic algorithm with stochastic ones. We start by looking at

an example for small n.

Example 15. *Let $n = 4$. We consider a vector of covariances given by*

$$R = \begin{pmatrix} 1 & 0.1 & 0.2 & 0.2 \\ 0.1 & 1 & 0.25 & 0.4 \\ 0.2 & 0.25 & 1 & 0.3 \\ 0.2 & 0.4 & 0.3 & 1 \end{pmatrix}$$

We know that the corresponding correlation matrix is realizable. We want to find a λ, that would give a measure that realizes R. We start with an initial λ given by

$$\lambda_0 = \begin{pmatrix} 1 & 0.5 & 0 & 0 \\ 0.5 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Following the notations in the algorithms we denote by u, the sample covariance matrix.

- *Deterministic Algorithm. We get the final vector of covariances as*

$$R^* = \begin{pmatrix} 1 & 0.1 & 0.2 & 0.2 \\ 0.1 & 1 & 0.25 & 0.4 \\ 0.2 & 0.25 & 1 & 0.3 \\ 0.2 & 0.4 & 0.3 & 1 \end{pmatrix}, \quad \lambda = \begin{pmatrix} 1 & 0.0000 & -0.1590 & -0.1590 \\ 0.0000 & 1 & -0.1658 & -0.3835 \\ -0.1590 & -0.1658 & 1 & -0.2245 \\ -0.1590 & -0.3835 & -0.2245 & 1 \end{pmatrix}$$

  in 1.5 seconds. The plot of λ_{12} with time looks like:

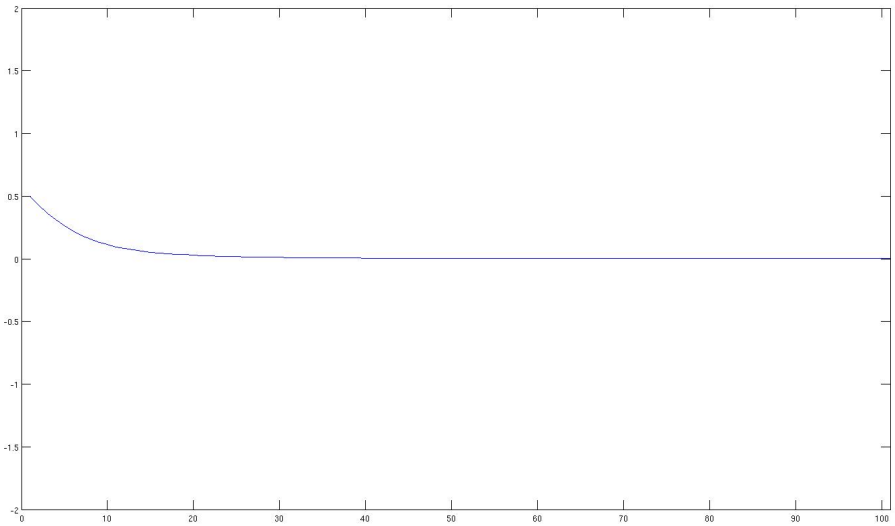

FIGURE 5.7.3: n = 4, discrete deterministic algorithm, no. of time steps = 100

- *MCMC algorithm yields*

$$u = \begin{pmatrix} 1.0000 & 0.0961 & 0.2003 & 0.2124 \\ 0.0961 & 1.0000 & 0.2505 & 0.3950 \\ 0.2003 & 0.2505 & 1.0000 & 0.2998 \\ 0.2124 & 0.3950 & 0.2998 & 1.0000 \end{pmatrix}$$

$$R^* = \begin{pmatrix} 1.000 & 0.1001 & 0.1990 & 0.1984 \\ 0.1001 & 1.0000 & 0.2514 & 0.4014 \\ 0.1990 & 0.2514 & 1.0000 & 0.2968 \\ 0.1984 & 0.4014 & 0.2968 & 1.0000 \end{pmatrix}$$

with

$$\lambda = \begin{pmatrix} 1.000 & 0.0008 & -0.1578 & -0.1567 \\ 0.0008 & 1.0000 & -0.1690 & -0.3850 \\ -0.1578 & 0.1690 & 1.0000 & -0.2201 \\ -0.1567 & 0.3850 & 0.2201 & 1.0000 \end{pmatrix}$$

in $T \approx 2113$ *seconds. The evolution of* λ_{12} *with time is as follows:*

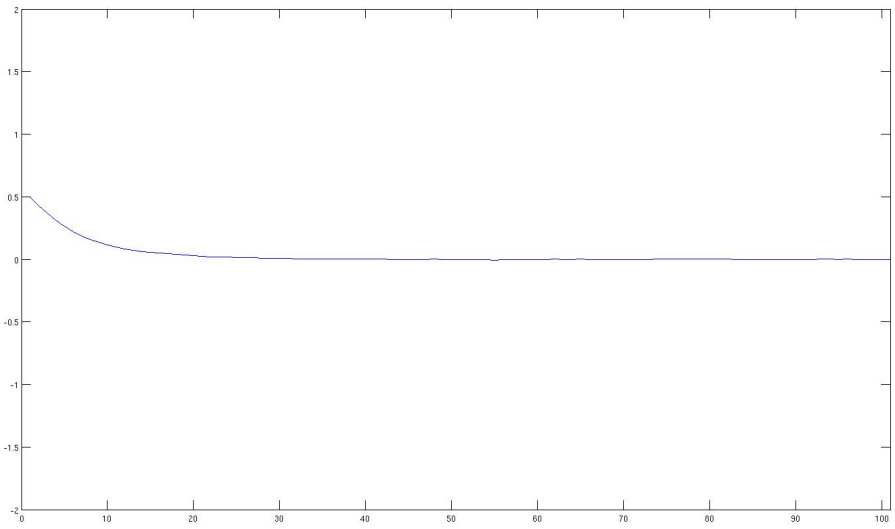

FIGURE 5.7.4: n = 4, MCMC, no. of time steps = 100, Markov chain steps = 100000

- *MCMC with geometric update*

  For the same parameter, MCMC with geometric update takes ≈ 2000 *seconds. The evolution of* λ_{12} *with time is as follows:*

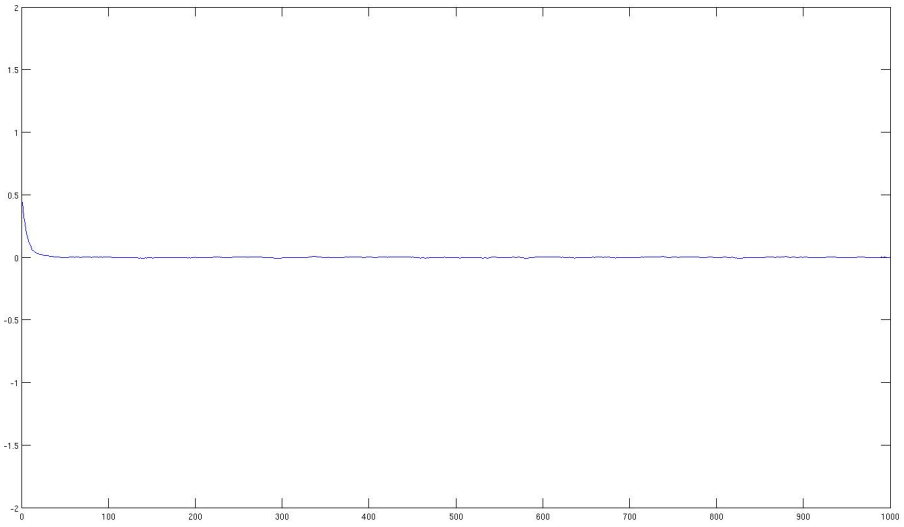

FIGURE 5.7.5: n = 4, MCMC with geometric update

- *Adaptive MCMC*

$$u = \begin{pmatrix} 1.0000 & 0.0990 & 0.1993 & 0.1999 \\ 0.0990 & 1.0000 & 0.2506 & 0.3989 \\ 0.1993 & 0.2506 & 1.0000 & 0.2990 \\ 0.1999 & 0.3989 & 0.2990 & 1.0000 \end{pmatrix}$$

and,

$$\lambda = \begin{pmatrix} 1.0000 & -0.1063 & -0.1876 & -0.1511 \\ 0.1063 & 1.0000 & -0.1846 & -0.3720 \\ -0.1876 & -0.1846 & 1.0000 & -0.2330 \\ -0.1511 & -0.3720 & -0.2330 & 1.0000 \end{pmatrix}$$

in $T \approx 367$ *seconds. The evolution of* λ_{12} *with time is as follows:*

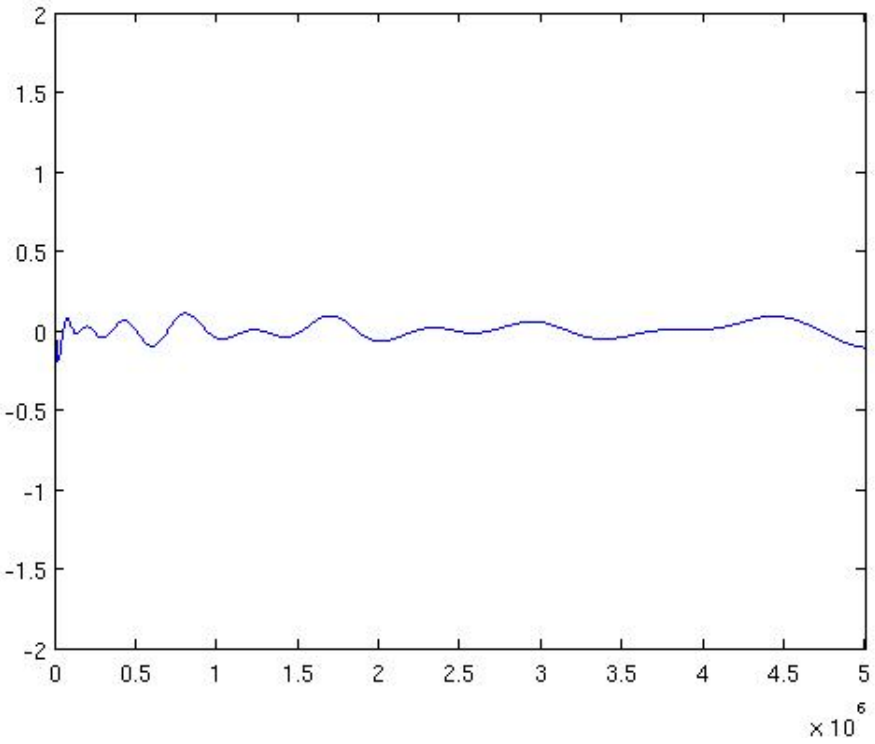

FIGURE 5.7.6: n = 4, adaptive MCMC, no. of time steps = 5000000

- *Adaptive MCMC: Modification I*

$$u = \begin{pmatrix} 1.0000 & 0.0981 & 0.1994 & 0.1986 \\ 0.0981 & 1.0000 & 0.2484 & 0.3983 \\ 0.1994 & 0.2484 & 1.0000 & 0.2977 \\ 0.1986 & 0.3983 & 0.2977 & 1.0000 \end{pmatrix}$$

and,

$$\lambda = \begin{pmatrix} 1.0000 & -0.0359 & -0.1667 & -0.1522 \\ -0.0359 & 1.0000 & -0.1285, -0.4112 & \\ -0.1667 & -0.1285 & 1.0000 & -0.2887 \\ -0.1522 & -0.4112 & -0.2887 & 1.0000 \end{pmatrix}$$

in $T \approx 1182$ *seconds. The evolution of* λ_{12} *with time is as follows:*

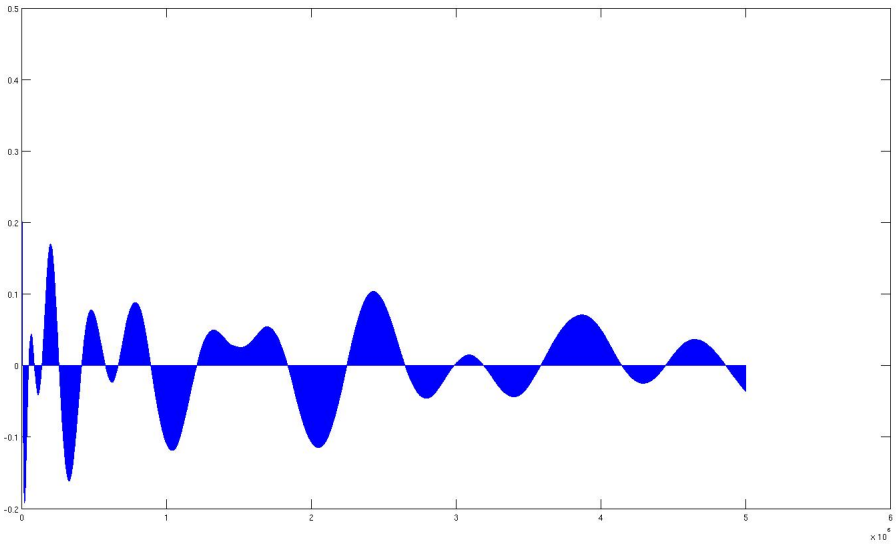

FIGURE 5.7.7: n = 4, Adaptive MCMC (Modification I), no. of time steps = 5000000, update after every 1000 steps

- *Adaptive MCMC: Modification II*

$$u = \begin{pmatrix} 1.0000 & 0.1006 & 0.2022 & 0.2009 \\ 0.1006 & 1.0000 & 0.2520 & 0.4016 \\ 0.2022 & 0.2520 & 1.0000 & 0.3023 \\ 0.2009 & 0.4016 & 0.3023 & 1.0000 \end{pmatrix}$$

and,

$$\lambda = \begin{pmatrix} 1.0000 & -0.0028 & -0.1682 & -0.2027 \\ -0.0028 & 1.0000 & -0.1912 & -0.3664 \\ -0.1682 & -0.1912 & 1.0000 & -0.3239 \\ -0.1993 & -0.3664 & -0.3239 & 1.0000 \end{pmatrix}$$

in $T \approx 726$ seconds. The evolution of λ_{12} with time is as follows:

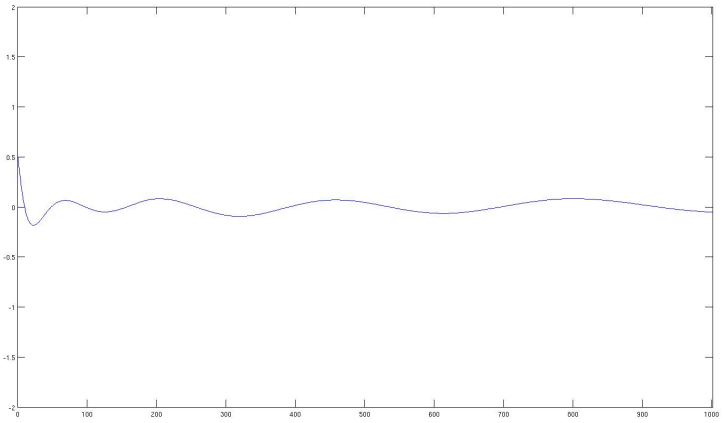

FIGURE 5.7.8: n = 4, Adaptive MCMC (Modification II)

Looking at the results, it is clear that while convergence of λ is rather slow, the sample covariances u edge close to the input R much faster.

Clearly the deterministic algorithms are much better for small n because it takes some time for the Markov chain to converge. However, since the deterministic algorithms involve calculating exponentials very often, it is expected that the stochastic algorithms yield much better results (in terms of time consumed) for sufficiently large n. This can be illustrated by considering the same problem for a large n.

Example 16. *Let us consider an example for $n = 10$. Let*

$$A = \begin{pmatrix} 1 & 0.1 & 0.2 & 0.3 & 0.1 \\ 0.1 & 1 & 0.25 & 0.4 & 0.1 \\ 0.2 & 0.25 & 1 & 0.3 & 0.1 \\ 0.3 & 0.4 & 0.3 & 1 & 0.1 \\ 0.1 & 0.1 & 0.1 & 0.1 & 1 \end{pmatrix}$$

We then consider the correlation matrix

$$R = \left(\begin{array}{c|c} A & \mathcal{O} \\ \hline \mathcal{O} & A \end{array}\right)$$

where $\mathcal{O}$ denotes a 5×5 zero-matrix.

Let us look at the plot of λ_{12} for different algorithms in this case.

Deterministic:

This takes ≈ 40932 seconds to get to the precise fixed point λ. The plot of λ_{12} which is given by:

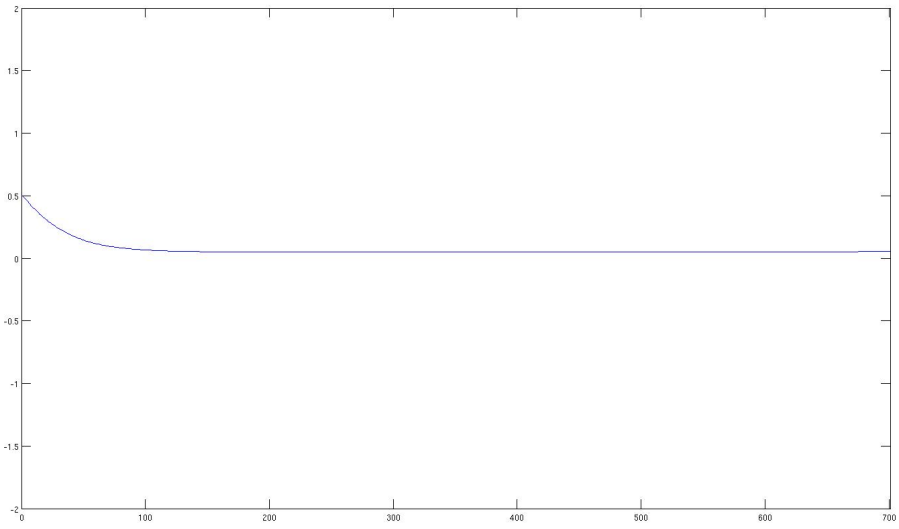

FIGURE 5.7.9: n = 10, Deterministic, 700 steps

$$\begin{pmatrix}
1.0000 & 0.0533 & -0.1337 & -0.2900 & -0.0723 & -0.0000 & -0.0000 & -0.0000 & 0.0000 & 0.0000 \\
.... & -0.1681 & -0.3948 & -0.0649 & -0.0000 & -0.0000 & -0.0000 & -0.0000 & 0.0000 & 0.0000 \\
... & ... & 1.0000 & -0.2083 & -0.0600 & 0.0000 & -0.0000 & -0.0000 & -0.0000 & 0.0000 \\
... & ... & ... & 1.0000 & -0.0358 & 0.0000 & -0.0000 & 0.0000 & 0.0000 & 0.0000 \\
... & ... & ... & ... & 1.0000 & -0.0000 & -0.0000 & -0.0000 & -0.0000 & 0.0000 \\
... & ... & ... & ... & ... & 1.0000 & 0.0532 & -0.1336 & -0.2898 & -0.0723 \\
... & ... & ... & ... & ... & ... & 1.0000 & -0.1681 & -0.3946 & -0.0649 \\
... & ... & ... & ... & ... & ... & ... & 1.0000 & -0.2084 & -0.0600 \\
... & ... & ... & ... & ... & ... & ... & .... & 1.0000 & -0.0358 \\
... & ... & ... & ... & ... & ... & ... & ... & ... & 1.0000
\end{pmatrix}$$

In comparison, the stochastic algorithms are faster.

MCMC:

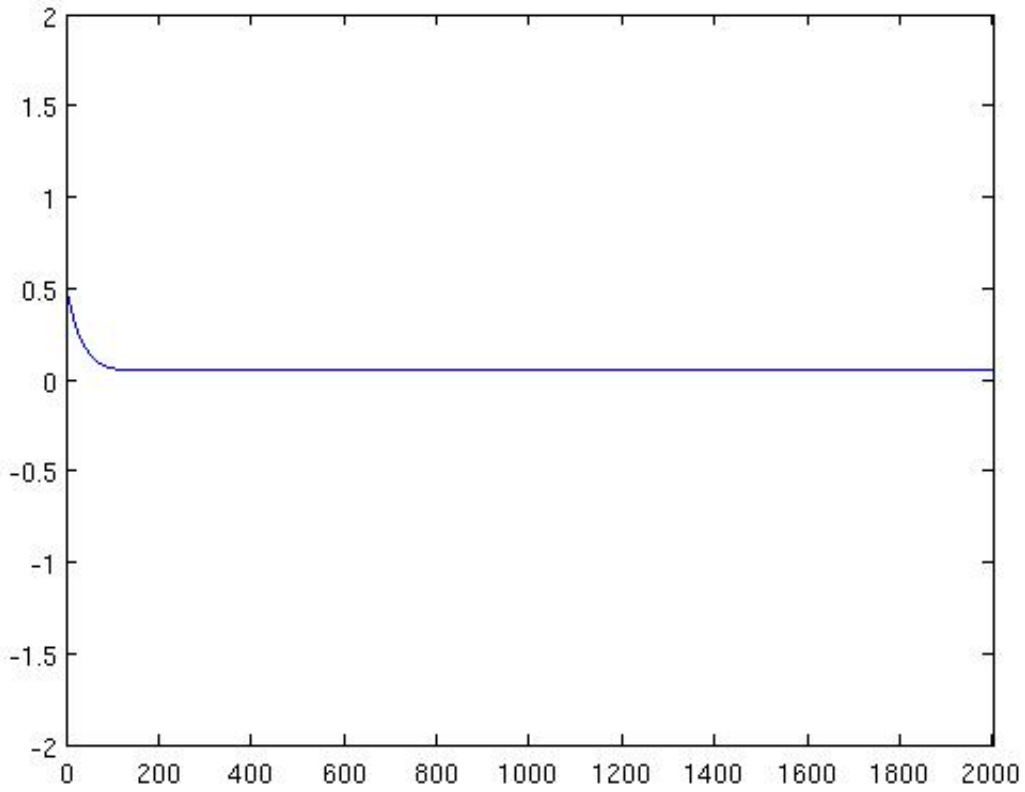

FIGURE 5.7.10: n = 10, MCMC, 2000 steps

Time taken is ≈ 22525 *seconds and the plot of* λ_{12} *which is given by:*

$$\begin{pmatrix} 1.0000 & 0.0517 & -0.1320 & -0.2908 & -0.0711 & -0.0014 & -0.0004 & -0.0007 & 0.0001 & 0.0003 \\ .... & -0.1701 & -0.3955 & -0.0642 & -0.0008 & -0.0015 & -0.0014 & -0.0006 & 0.00023 & 0.0017 \\ ... & ... & 1.0000 & -0.2081 & -0.0570 & 0.0014 & -0.0004 & -0.0008 & -0.0008 & 0.0021 \\ ... & ... & ... & 1.0000 & -0.0340 & 0.0021 & -0.0036 & 0.0012 & 0.0028 & 0.0034 \\ ... & ... & ... & ... & 1.0000 & -0.0011 & -0.0012 & -0.0025 & -0.0031 & 0.0027 \\ ... & ... & ... & ... & ... & 1.0000 & 0.0528 & -0.1384 & -0.2831 & -0.0725 \\ ... & ... & ... & ... & ... & ... & 1.0000 & -0.1686 & -0.3966 & -0.0644 \\ ... & ... & ... & ... & ... & ... & ... & 1.0000 & -0.2065 & -0.0587 \\ ... & ... & ... & ... & ... & ... & ... & .... & 1.0000 & -0.0345 \\ ... & ... & ... & ... & ... & ... & ... & ... & ... & 1.0000 \end{pmatrix}$$

MCMC with geometric updating

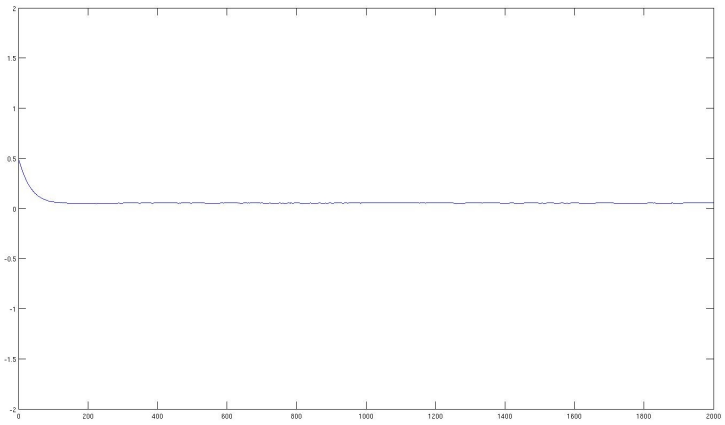

FIGURE 5.7.11: n = 10, MCMC with geometric updating, 2000 steps

Time taken is ≈ 22697 *seconds and the plot of* λ_{12} *which is given by:*

$$\begin{pmatrix}
1.0000 & 0.0553 & -0.1341 & -0.2901 & -0.0722 & -0.0000 & -0.0005 & -0.0010 & 0.0017 & 0.0021 \\
.... & -0.1692 & -0.3923 & -0.0636 & -0.0006 & -0.0004 & -0.0023 & -0.0002 & 0.0002 & 0.0010 \\
... & ... & 1.0000 & -0.2095 & -0.0615 & 0.0004 & -0.0002 & -0.0001 & -0.0009 & 0.0022 \\
... & ... & ... & 1.0000 & -0.0357 & 0.0017 & -0.0007 & 0.0001 & 0.0006 & 0.0003 \\
... & ... & ... & ... & 1.0000 & -0.0014 & -0.0002 & -0.0015 & -0.0012 & 0.0005 \\
... & ... & ... & ... & ... & 1.0000 & 0.0531 & -0.1341 & -0.2898 & -0.0721 \\
... & ... & ... & ... & ... & ... & 1.0000 & -0.1675 & -0.3933 & -0.0661 \\
... & ... & ... & ... & ... & ... & ... & 1.0000 & -0.2066 & -0.0601 \\
... & ... & ... & ... & ... & ... & ... & .... & 1.0000 & -0.0371 \\
... & ... & ... & ... & ... & ... & ... & ... & ... & 1.0000
\end{pmatrix}$$

One can see, that because of geometric updating, even though the time taken for the same number of loops is same, the convergence is slightly faster and λ *obtained is closer to the fixed point, than the one obtained by pure MCMC.*

Adaptive MCMC:

Time taken is ≈ 11665 *seconds.*

Even though the λ *seems to oscillate, it remains inside the small neighbourhood and the the sample covariance* u *obtained in the end is considerably close to* R*.*

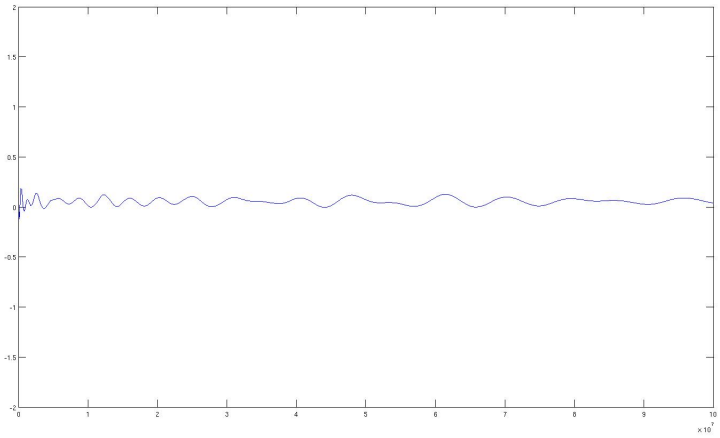

FIGURE 5.7.12: n = 10, Adaptive MCMC, 100000000 steps

$$u = \begin{pmatrix} 1.0000 & 0.0996 & 0.2006 & 0.2995 & 0.0993 & 0.0000 & -0.0002 & -0.0005 & 0.0000 & 0.0003 \\ .... & 1.0000 & 0.2503 & 0.3996 & 0.0988 & -0.0002 & 0.0001 & -0.0002 & 0.0009 & 0.0004 \\ ... & ... & 1.0000 & 0.2994 & 0.1003 & 0.0006 & -0.0001 & 0.0005 & 0.0005 & 0.0009 \\ ... & ... & ... & 1.0000 & 0.0993 & 0.0011 & -0.0012 & -0.0010 & 0.0004 & -0.0000 \\ ... & ... & ... & ... & 1.0000 & -0.0003 & -0.0012 & -0.0006 & -0.0007 & 0.0001 \\ ... & ... & ... & ... & ... & 1.0000 & 0.1001 & 0.2002 & 0.3001 & 0.0993 \\ ... & ... & ... & ... & ... & ... & 1.0000 & 0.2505 & 0.4002 & 0.0998 \\ ... & ... & ... & ... & ... & ... & ... & 1.0000 & 0.2993 & 0.0999 \\ ... & ... & ... & ... & ... & ... & ... & .... & 1.0000 & 0.1010 \\ ... & ... & ... & ... & ... & ... & ... & ... & ... & 1.0000 \end{pmatrix}$$

Adaptive (Modification I)

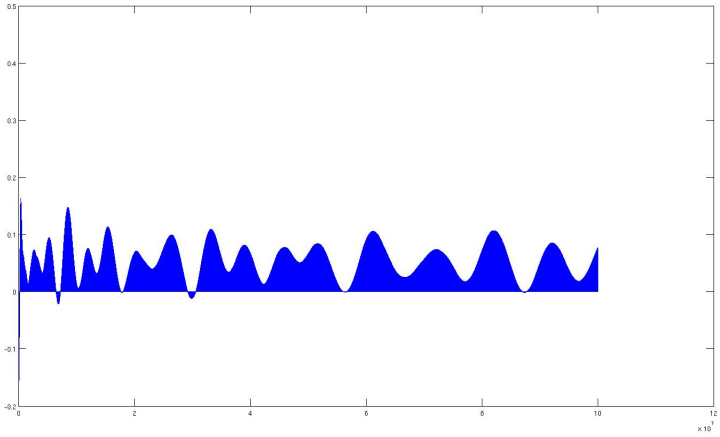

FIGURE 5.7.13: n = 10, Adaptive MCMC (Modification I)

Adaptive (Modification II)

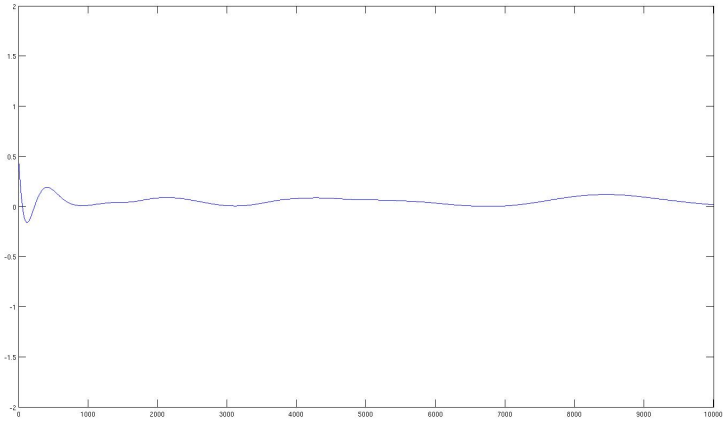

FIGURE 5.7.14: n = 10, Adaptive MCMC (Modification II)

Let us consider a slightly larger n. For $n = 12$, we consider the following matrix of covariances:

$$R = \left(\begin{array}{c|c|c|c} A & A & A & A \\ \hline A & A & A & A \\ \hline A & A & A & A \\ \hline A & A & A & A \end{array}\right), \quad \text{where } A = \begin{pmatrix} 1 & 0.1 & 0.2 \\ 0.1 & 1 & 0.1 \\ 0.2 & 0.1 & 1 \end{pmatrix}$$

The deterministic algorithm in this case is extremely slow. One step (for updating λ) takes 2580 seconds. Since the deterministic algorithm requires more than 600 steps to converge, the total time takes is very large (> 400 hours!). The MCMC algorithm is comparatively quicker. For the deterministic algorithm, time taken for executing one step, that is, for one update of λ is $0.707, 0.196, 6.044, \approx 120$ and 2238 seconds for $n = 4, 5, 8,$ various matrices of size 10 and 12 respectively. On the other hand, the time taken for MCMC algorithm (both the usual MCMC and the one with geometric updating) increases from 7 to 15 seconds as we go from $n = 4$ to $n = 12$. The same holds true for the modifications of the adaptive algorithm.This means that it is clearly more useful to use the MCMC based methods for large n.

The time taken by the deterministic algorithms increases rapidly with increasing n. Hence, they are not very useful for problems involving large number of spins. For large n, the MCMC algorithm can be used to approximate the correct λ.

Chapter 6

Further Applications and Ideas

6.1 Quantum Spins

6.1.1 Setting

We define Quantum spins as follows. In correspondence with the classical spin values ± 1, we consider the two dimensional vectors

$$|\ 1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad\qquad |-1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

The pair $|\ 1\rangle$ and $|-1\rangle$ is a basis of the state space for a one-site quantum spin system, provided with the Euclidean scalar product. For a finite $\Lambda \subseteq \mathbb{Z}^d$, we consider the classical spin system $\Omega^\Lambda = \{-1, 1\}^\Lambda$. The corresponding quantum space is given by

$$\mathbb{X}_\Lambda \otimes_{i\in\Lambda} \mathbb{C}^2$$

We denote by $|\sigma\rangle = \otimes_{i\in\Lambda}|\sigma_i\rangle$ the $2^{|\Lambda|}$ elements of a basis of $\mathbb{X}_\Lambda$; the scalar product, defined on the elements of the basis by

$$\langle\sigma|\sigma'\rangle = \prod_{i\in\Lambda}\langle\sigma_i|\sigma'_i\rangle,\ i \in \Lambda$$

makes it into an orthonormal basis. Let now by $\hat{\sigma}^z$ the Pauli matrix,

$$\hat{\sigma}^z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and denote by $\hat{\sigma}_i^z$ the linear operator on $\mathbb{X}_\Lambda$ defined on the basis by

$$\hat{\sigma}_i^z|\sigma\rangle := |\sigma_1\rangle \otimes \ldots \otimes \hat{\sigma}^z|\sigma_i\rangle \otimes \ldots |\sigma_{|\Lambda|}\rangle. \tag{6.1.1}$$

Given a function $H : \Omega_\Lambda \to \mathbb{R}$, it can be lifted to the self-adjoint operator $\mathcal{H}_{cl}$ on $\mathbb{X}_\Lambda$ by

$$\mathcal{H}_{cl}|\sigma\rangle = H(\hat{\sigma}_1^z, \ldots, \hat{\sigma}_{|\Lambda|}^z)|\sigma\rangle = H(\sigma)|\sigma\rangle.$$

The models we consider are obtained by adding a *transverse field* to a given classical Hamiltonian $\mathcal{H}_{cl}$. To the Pauli matrix

$$\hat{\sigma}^x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

we associate, as in (6.1.1), the operators $\hat{\sigma}_i^x$. Given real numbers $\{l_i : i \in \Lambda\}$, we define the Hamiltonian

$$\mathcal{H} := \mathcal{H}_{cl} - \sum_{i\in\Lambda} l_i \hat{\sigma}_i^x. \tag{6.1.2}$$

It should be noticed that there is some arbitrariness in the choice of the basis $|\ 1\rangle, |-1\rangle$ of eigenvectors for $\hat{\sigma}^z$. For instance, if we transform the canonical choice given above to $|\ 1\rangle := \binom{-1}{0}$ and $|-1\rangle := \binom{0}{1}$, the corresponding change of variables would transform $\hat{\sigma}^x$ to $-\hat{\sigma}^x$. Since this choice can be made component-wise, we can always choose a basis of $\mathbb{X}_\Lambda$ such that the Hamiltonian corresponds to the matrix (6.1.2) with nonnegative values of the λ_i's. Thus without loss of generality we may assume that $\lambda_i \geq 0$ for every $i \in \Lambda$.

An observable $\mathcal{F}$ its *quantum average* is given by

$$< \mathcal{F} >:= \frac{Tr\mathcal{F}e^{-\beta\mathcal{H}}}{Tre^{-\beta\mathcal{H}}}.$$

Similarly, for two observables $\mathcal{F}$ and $\mathcal{G}$, the *(truncated) correlation* is defined by

$$< \mathcal{F}; \mathcal{G} >:=< \mathcal{F}\mathcal{G} > - < \mathcal{F} >< \mathcal{G} > .$$

To the classical observable $f : \Omega_\Lambda \to \mathbb{R}$, we associate the quantum counterpart

$$\mathcal{F}_f := f(\hat{\sigma}_1^z, \ldots, \hat{\sigma}_{|\Lambda|}^z).$$

For $\sigma \in \Omega_\Lambda$ and $i \in \Lambda$, σ^i denotes the element of Ω_Λ obtained from σ by flipping the i^{th} spin.

In the next section we will reformulate the stochastic-geometric representation of the Quantum

field defined here. This would allow us to view quantum means and correlations of observables as classical means and correlations with respect to a suitable distribution π on a product space of marked point processes.

6.1.2 Stochastic Geometric Representation

We denote by Δ the set of piecewise constant, right continuous functions from $[0,\beta) \to \{-1,1\}$, where $[0,\beta)$ is meant to be a circle ($0 = \beta$). This set is provided with the Skorohod topology. Moreover, Σ is the set of finite subsets of $[0,\beta)$. The topology on Σ is generated by the following sets, parametrized by $\eta \in \Sigma$ and $\epsilon > 0$: $\{\eta' \in \Sigma : |\eta'| = |\eta| \text{ and } dist(\eta,\eta') < \epsilon\}$, where $dist(\eta,\eta')$ denotes the Hausdorff distance between two sets. Finally, we define

$$S := (\Delta \times \Sigma)^{\Lambda},$$

and provide it with the product topology.

If $\eta \in \Sigma$ and $a \in \Delta$, we say that $a \sim \eta$ (a is compatible with η) if the discontinuity points of a are a subset of η. Similarly, for $\xi \in \Sigma^{\Lambda}$ and $\sigma \in \Delta^{\Lambda}$ we write, by slight abuse of notation, $\sigma \sim \xi$ if $\sigma_i \sim \xi_i$ for every $i \in \Lambda$. We will sometimes say that σ is a *coloring* of ξ.

By P_i, $i \in \Lambda$, we denote the Poisson point measure on Σ with intensity l_i. By $\mathbb{P}$ we mean the product measure on Σ^{Λ}

$$\mathbb{P} = \otimes_{i\in\Lambda} P_i.$$

Consider the probability measure on S given by

$$\pi(\sigma, d\xi) := \frac{1}{Z}\mathbf{1}_{\{\sigma\sim\xi\}} \exp\left[\int_0^{\beta} H(\sigma_t)dt\right] \mathbb{P}(d\xi) \tag{6.1.3}$$

where Z is a normalization factor. Given Borel measurable functions $\Phi, \Psi : S \to \mathbb{R}$, we denote by

$$\pi[\Phi] \quad \text{or} \quad \pi[\Phi(\sigma,\xi)]$$

the mean of Φ with respect to π, and by

$$\pi[\Phi;\Psi] \quad \text{or} \quad \pi[\Phi(\sigma,\xi);\Psi(\sigma,\xi)]$$

their covariance $\pi[\Phi\Psi] - \pi[\Phi]\pi[\Psi]$.

6.1.3 A covariance realization problem for Quantum spins

Theorem 6.1.1. *[9] Let $f, g : \Omega_{\Lambda} \to \mathbb{R}$. Then,*

$$\begin{aligned} \langle \mathcal{F}_f \rangle &= \pi[f(\sigma_0)] \\ \langle \mathcal{F}_f, \mathcal{F}_g \rangle &= \pi[f(\sigma_0), g(\sigma_0)] \end{aligned} \tag{6.1.4}$$

where Ω_Λ is as defined in section 6.1.1.

As mentioned before, this theorem allows us to consider a covariance realization problem for the Quantum Spin system defined in section 6.1.1 as a covariance realization problem for the system of classical spins given by σ_0 in accordance with the description given in the previous section.

Consider a probability measure of the form given in (6.1.3). The corresponding entropy function is give by

$$S(\pi, \mathbb{P}) = -\int_S \pi(\sigma, d\xi) \log \frac{\pi(\sigma, d\xi)}{\mathbb{P}(d\xi)} \tag{6.1.5}$$

We impose the covariance constraints:

$$\int_S \sigma_t(i)\pi(\sigma, d\xi) = 0 \quad \forall\, t, i$$
$$\int_S \sigma_t(i)\sigma_t(j)\pi(\sigma, d\xi) = c_{ij}$$

We consider the corresponding maximum (classical) entropy problem. We want to find a Hamiltonian $H(\sigma_t)$ that maximizes the entropy subject to the above stated constraints. The Lagrange function as defined in chapter 3, section 3.2.1, is of the form

$$\mathcal{L}(\pi, \lambda) = S(\pi, \mathbb{P}) + \sum_{ij} \int \int_0^\beta \sigma_t(i)\sigma_t(j)\lambda_{ij}(t)\pi(\sigma, d\xi)dt \tag{6.1.6}$$

Then, doing the calculations that resemble the Lagrange multiplier method used in section 3.2.2 for classical spin system, we get,

$$\frac{d\pi}{d\mathbb{P}} = \frac{1}{Z} \exp\left[\sum_{ij} \int_0^\beta \sigma_t(i)\sigma_t(j)\lambda_{ij}(t)dt\right]$$

Or,

$$d\pi = \frac{1}{Z} \exp\left[\sum_{ij} \int_0^\beta \sigma_t(i)\sigma_t(j)\lambda_{ij}(t)dt\right] d\mathbb{P}$$

Notice, that the Hamiltonian $H(\sigma_t)$ is independent of β. This means that the corresponding conditions for feasibility of the problem are the same as obtained in chapter 3, section 3.2.2.

This is rather interesting because this means that the necessary and sufficient conditions obtained

in Chapter 3 can be used for a Quantum system (as described above) as well. This places the problem of covariance realization for spins in a much larger and interesting context.

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