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A CAVITY ALGORITHM FOR OPTIMAL ASSIGNMENT

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# Introduction

Studies on disordered systems in Statistical Mechanics, like spin glasses and random models, have developed and refined in the last thirty years a set of sophisticated and useful means for dealing with a wide range of complex phenomena, the Replica and the Cavity Methods being paradigmatic examples of these elaborate tools. These, in turn, opened new ways for representing and understanding the complexity coming out in a lot of subjects of research, not only as far as physical matters are concerned.

Combinatorial Optimization is certainly one of the natural field in which such developments could be applied. So it is not surprising that one of the first accounts of such methods [1] devoted one section to the applications in optimization problems.

Combinatorial Optimization deals with the search and the analysis of effective algorithms for selecting objects in a huge space of feasible solutions given some variational principles. Here we highlight the good scaling properties with the “size” of the problem, mainly in the worst case scenario. Algorithms are then classified in a hierarchic manner in some complexity class.

While the Statistical Mechanics of disordered systems tries, through a probabilistic approach, to catch a qualitative and structural picture of the whole space of configurations, here we focus on the features of different models that show some “universality” properties.

Although the somewhat different aims of these two fields, a lot of problems could be stated in a very unified presentation, and the results of one discipline could be frequently transposed in the proper language of the other one, leading to a fruitful interplay.

This work picks up a classical subject of Combinatorial Optimization, the Assignment Problem, and tries to design and analyze for it an algorithm inspired to the Cavity approach on the related Statistical Mechanical model. The Assignment Problem consists in finding a minimum weight matching in a weighted bipartite graph, i.e., loosely speaking, given a cost for every pairs between two set of objects of equal size  $N$ ; the problem consists in selecting  $N$  pairs so that the sum of their cost is minimal and each object is in one and only one pair.

This problem is worth of study for different reasons, among which we can mention the practical applications related to the switching technology and the image pattern recognition. Another interesting feature is certainly the polynomial time boundedness of available algorithms for this

problem, that allows a controllable testing of the physical expectations for this model.

Using the Cavity Theory for Random Models we investigated finite-size behaviour in order to design a competitive algorithm for optimal assignment given a random matrix. From Cavity Equations for this model we derived a recursive map for “bias” fields. Some interesting features came out:

- a fixed point exists almost everywhere in the measure for the cost matrix using a parallel update for the fields;
- such fixed point is a delta function over the optimal configuration
- the attraction basin of this solution covers all the space of initial values for bias fields.

Thus an exact algorithm is extracted from the Cavity Method for solving the random Assignment Problem. Similar analyzes are also found in [2], but some practical aspects for the algorithm design are not addressed there. For example they do not provide an *a priori* (i.e., instance independent) limit for the solution time. Also it lacks a criterion for asserting that the fields are sufficiently “close” to the asymptotic behaviour. Finally naïve solution time averages are infinite because of non-integrable power tail distribution over the instances.

A well-known algorithm for Assignment Problem (*Hungarian* Algorithm, [3]) was studied in order to underline similarities and differences with the Cavity algorithm, and through its study it was possible to derive a solution certification for the Cavity algorithm.

A heuristic for determining instances with anomalous long time convergence and an *ad hoc* prescription for dealing with them were developed in order to get a total computing time law close to the cubic power law of the Hungarian Algorithm.

Some remarks are also discussed for the practical use of the Cavity algorithm. Even though the Hungarian Algorithm behaves comparatively better as regards solution time, the cavity approach could give fast sub-optimal heuristic, and it is easier to implement in a parallel architecture.

The chapter structure is as follows:

- Chapter 1 deals with the typical phenomena of the random systems in Statistical Mechanics. It is a brief account of concepts and techniques often used in the other chapters.
- Then in chapter 2, some ideas from the Combinatorial Optimization are presented such as the hierarchic structure of the complexity classes and it is described in some details a polynomial algorithm for this problem: the Hungarian Algorithm.
- In chapter 3 we give a better look at the Cavity Method for the Random Assignment Problem, leading to the recursive map used in the algorithm.

- In chapter 4 is contained the finite-size analysis of the model, and some implementation details are discussed together with the Belief Propagation interpretation for the Cavity Algorithm. Finally it is discussed in some length the Replica Symmetry for our model.
- Chapter 5 contains the main demonstration of the convergence and of the features emerging in the stationary phase for the iterative map. A central discussion covers also the theoretical basis for the halting condition and the optimality certificate.
- In chapter 6 are faced some important aspects for raising the heuristics described in the previous chapters to an algorithm, and it is also analyzed the scaling properties of the efficiency of the algorithm.
- Finally is included a “conclusion and perspective” chapter for discussing and resuming the results.



# Chapter 1

## Introduction to concepts of Statistical Mechanics

This chapter is a brief introduction to the concepts of disordered systems in Statistical Mechanics. It is mainly intended for people who lack familiarity with these fields, for example because they come from a background in Computer Science. So, it is absolutely non-exhaustive, but we hope that we succeeded in giving a flavour of the main concepts, with a special eye to those points which will be reanalyzed, in a refined way, in the following chapters. Clearly, the reader familiar with the theory of Spin Glasses can skip reading this part.

First, the general framework of equilibrium Statistical Mechanics will be presented; then we will concentrate on the archetypal Ising Model, in order to introduce the subtle concepts of spontaneous symmetry breaking and phase transition through a pictorial example. Finally, some models of disordered systems are presented, and some attempt to describe the arising new features is done.

### 1.1 Equilibrium Statistical Mechanics

The core subject of Statistical Mechanics is the bridge, built with probabilistic tools, between the macroscopic world of Thermodynamics and the microscopic one, which it is believed to obey to some elementary physical law, such as those of Mechanics.

Its reductionist research program started in the eighteenth century with the works of Boltzmann, Maxwell, Gibbs and others, in order to “explain” the thermodynamic laws empirically observed since the seventeenth century (such as the classical ideal gas law) as macroscopic effects of an underlying micro-physics of “atoms” subject to the laws of Newtonian Mechanics.

The microscopic state of a thermodynamic system could not be accessed directly through

measurements. Experiments can only gather statistical data concerning the system as a macrostate, and repeat measure procedures on a physical state prepared in a well defined manner (i.e., imposing a finite set of thermodynamic and boundary condition such as pressure, volume, temperature, external magnetic field...).

As they were facing both the impossibility of fixing the microphysical state through measurements, and the overwhelming difficulties in solving the equation of motion for a huge number of coupled degrees of freedom, statistical mechanicians were forced in the use of a probabilistic approach.

Assuming that the relevant properties of a particle (such as position, momentum, spin, ...) are described in a *single-state space*  $X_0$ , the microscopic state is fully described by an unknown point in a high-dimensional phase space  $X = X_0^N$  ( $N \sim 10^{23}$  on human-size experiments) provided with a reference measure  $dx$  inherited from the one over  $X_0$ . After the system preparation, including a transient time of *thermalization*, it is assumed that the system reaches the thermal equilibrium, then a measure  $d\mu^{(P,V,T,\dots)}$  (depending on a finite set of thermodynamic conditions) describes the physical system subjected to measurements.

Observable quantities correspond to real-valued functions over the phase space and their average values over the equilibrium measure lead to quantities amenable of experimental comparison.

$$A : X \rightarrow \mathbb{R}, \quad \langle A \rangle_\mu = \int_X d\mu(x) A(x)$$

For homogeneous systems, with short-range interactions (i.e. such that particles well in the bulk do not “feel” the boundary), it is expected that the local properties of the system in the bulk do not depend sensibly from the volume. For example, some water, at a given temperature and pressure, will have a certain density  $\rho$  regardless from the size and shape of the container. Similarly, the mass  $M$  of water in the container will be proportional to the volume itself,  $M = \rho V$ . This trivial scaling reasonings allow to distinguish physical observables into *intensive*, not scaling with the volume, like the density, and *extensive*, scaling linearly with the volume, like the mass.

The microscopic equation of motion is involved through the Hamiltonian function  $\mathcal{H}$  that represents the energy of the system and generates trajectories of the microstate in the phase space. However, for reasons illustrated in the following, it makes sense to avoid a detailed description of the microscopic dynamics, and introduce instead models of Statistical Mechanics with simplified Hamiltonians. Nonetheless, in this step one should preserve some requirements on the Hamiltonian function based on physical grounds, such as locality and microscopic time-reversal symmetry, where the latter is automatically implemented by respecting the *detailed balance*: if  $W_{x \rightarrow x'}$  is the *transition rate* i.e., the probability that a microscopic configuration  $x$

evolves to the state  $x'$  after some time  $\Delta t$ , the dynamics has the following properties:

$$\lim_{|x-x'|\rightarrow\infty} W_{x\rightarrow x'} = 0 \quad (\text{locality}) \quad (1.1)$$

$$\frac{W_{x\rightarrow x'}}{W_{x'\rightarrow x}} = e^{-\beta(\mathcal{H}(x')-\mathcal{H}(x))} \quad (\text{detailed balance}) \quad (1.2)$$

In this picture, the task of Statistical Mechanics can be divided in two parts: on the one hand, to derive the probability measure of the system at thermal equilibrium (i.e., after a sufficient long time); on the other hand, to compute, even if in an approximate way, the macroscopic properties as averages over that measure.

The determination of the equilibrium measure  $d\mu^{(V,P,T,\dots)}$ , given the Hamiltonian, is in general a delicate point. Nevertheless, under the ergodic hypothesis, which roughly states that the trajectories in the phase space under the dynamics cover uniformly the equilibrium measure, or, equivalently, that time averages coincides asymptotically with averages over the measure

$$\langle A \rangle_\mu = \int_X d\mu(x) A(x) = \lim_{T\rightarrow\infty} \int_0^T dt A(x(t)) \quad \forall \text{ observable } A \quad (1.3)$$

it can be proved the existence of a unique equilibrium measure, i.e., the Gibbs measure for a system in a heat bath at temperature  $T \propto \frac{1}{\beta}$ :

$$d\mu^{\text{Gibbs}}(x) = \frac{e^{-\beta\mathcal{H}(x)}}{\mathcal{Z}(\beta)} dx \quad (1.4)$$

The failure of this hypothesis is the core of crucial concepts like spontaneous symmetry breaking, as we will discuss in the following. One should however distinguish among the “simple” mechanisms, deducible *a priori*, such as the existence of some other conserved quantity (besides energy), which determine a family of equilibrium measures, not parametrized by macroscopic external conditions, and some more “structural” mechanism, such that the ergodicity is broken by some large-volume limit of the dynamics, where the times required in (1.3) diverges with some exponential of the volume.

In the Gibbs measure above,  $\mathcal{Z}(\beta)$  is the *partition function*. Algebraically it expresses the normalization of the measure:

$$\mathcal{Z}^{\text{Gibbs}}(\beta) = \int_X dx e^{-\beta\mathcal{H}(x)} \quad (1.5)$$

while its physical meaning comes from the following simple relations for the mean energy and its thermal fluctuations:

$$E(\beta) = \langle \mathcal{H} \rangle_\mu = -\frac{\partial}{\partial \beta} \ln(\mathcal{Z}(\beta))$$

$$\langle \mathcal{H}^2 \rangle_\mu - \langle \mathcal{H} \rangle_\mu^2 = \frac{\partial^2}{\partial \beta^2} \ln(\mathcal{Z}(\beta))$$

Let us remark some important properties of generic Statistical Mechanics systems:

- given a set of non-interacting systems  $X_1, X_2, \dots, X_k$  (i.e., uncorrelated), the composite partition function is given by a product over the components:  $\mathcal{Z} = \prod_{i=1}^k \mathcal{Z}_i$ ;
- the logarithm of the partition function is an extensive quantity (i.e., proportional to the size of the system), and is called *free energy*:

$$\mathcal{F}(\beta) = -\frac{1}{\beta} \ln(\mathcal{Z}(\beta)) \quad (1.6)$$

Alongside with the free energy, another fundamental concept is the *entropy* of the system, defined as:

$$\mathcal{S}[\mu] = - \int_X d\mu(x) \ln(\mu(x)) = -\langle \ln \rangle_\mu \quad (1.7)$$

where we use square brackets to underline its aspect of functional over the space of measures in the phase space. Its exponential “measures” the number of relevant states in the phase space for the considered probability measure. The Gibbs measure satisfies the variational principle of maximal entropy at given mean energy, or the principle of maximal free energy, as it should be evident from the following relations for the entropy, the internal energy and the free energy:

$$\text{(entropy)} \quad \mathcal{S}[\mu] = -\langle \ln \rangle_\mu \quad (1.8)$$

$$\text{(internal energy)} \quad \mathcal{E}[\mu] = \langle \mathcal{H} \rangle_\mu \quad (1.9)$$

$$\text{(free energy)} \quad \mathcal{F}[\mu] = \mathcal{E}[\mu] - \frac{\mathcal{S}[\mu]}{\beta} \quad (1.10)$$

Moreover using the equilibrium measure it is possible to derive the following formulae

$$\mathcal{F}(\beta) = -\frac{1}{\beta} \ln(\mathcal{Z}(\beta)) \quad (1.11)$$

$$\mathcal{S}(\beta) = -\beta^2 \frac{\partial \mathcal{F}}{\partial \beta}(\beta) \quad (1.12)$$

$$\mathcal{E}(\beta) = \mathcal{F}(\beta) + \beta \frac{\partial \mathcal{F}}{\partial \beta}(\beta) \quad (1.13)$$

Looking at them it should be clear how a thermodynamic potential, such as the free energy, encodes much of the physics of the system. Furthermore, observables essentially of any nature can be expressed through the calculation of a partition function for a sufficiently “generalized” model, extended to include some source terms,

$$\langle A \rangle = -\frac{1}{\beta} \frac{\partial}{\partial j} \ln(\mathcal{Z}(\beta, j)) \Big|_{j=0}, \quad \mathcal{Z}(\beta, j) = \int_X dx e^{-\beta(\mathcal{H}(x)+jA(x))}. \quad (1.14)$$

## 1.2 Ordered Systems and Phase Transition

In this section we set out to give a brief overview on an archetypal toy model of ordered systems: the Ising Model, because it provides an insightful example of some recurrent features of Statistical Mechanics such as ergodicity breaking, phase transition and coexistence of pure phases.

Ernst Ising developed the model in 1926 as part of his PhD dissertation. The 1-dimensional Ising Model consists of a linear chain, made up of particles having magnetic moments called “spins” that are able to take an up or down position. The spin of each particle influences the spin moment of the ones bordering it.

More generally, let us consider a spin system on a  $d$ -dimensional regular lattice of size  $L$ , in which each site contains a spin variable  $\sigma$  whose values lie in the single-state space  $X_0 = \{\pm 1\}$ . The Hamiltonian function is:

$$\mathcal{H}(\boldsymbol{\sigma}) = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j + h \sum_i \sigma_i \quad (1.15)$$

where  $J$  represents the strength of the interaction between the sites of the lattice,  $\langle i,j \rangle$  means sum over nearest neighbours,  $h$  is a site-independent external magnetic field and  $\boldsymbol{\sigma} = \{\sigma_1, \sigma_2, \dots\}$  indicates the configuration of the microstate in the phase space  $X = \{\pm 1\}^N$  (with  $N = L^d$ ).

The calculation of the Gibbs partition function  $\mathcal{Z}_N$ :

$$\mathcal{Z}_N = \sum_{\boldsymbol{\sigma}} e^{-\beta \mathcal{H}(\boldsymbol{\sigma})} \quad (1.16)$$

results easy in 1-dimensional systems, but despite of a deceiving simplicity, its analytical treatment leads to serious difficulties even in the 2-dimensional case. This calculation was solved with no external magnetic field through a mathematical tour de force by Onsager in 1944 [4]. In higher dimensions other techniques should be tried, such as computer simulations (like Monte Carlo methods or Transfer Matrix techniques), or analytical approximations (like Low and High Temperature expansions, or a systematic Mean Field expansion of  $k$ -point correlation functions).

In order to get a qualitative picture of its behaviour, let us consider the natural observable of mean magnetization, defined as

$$M = \langle m(\boldsymbol{\sigma}) \rangle, \quad \text{with} \quad m(\boldsymbol{\sigma}) = \frac{1}{N} \sum_i \sigma_i \quad (1.17)$$

Obviously, if  $h = 0$ , the Gibbs measure leads to zero mean magnetization for each temperature, (disregarding thermal fluctuation) due to symmetry reasons. Nonetheless, if the dynamics selects a region of the phase space with (absolute value of) average magnetization  $|m(\boldsymbol{\sigma})| \sim m^*$ , we would have two “bubbles” in the phase space, each of them being ergodically explored in short times, but the “tunnelling” from one to the other, requiring that the system explores highly improbable

regions of the phase space for a large time, is possible in principle, but suppressed by factors  $\sim \exp(-\beta E)$  (with  $E$  some typical energy of this tunnelling process, which is extensive).

Performing an exact analytical computation of  $M(T, h)$  using the true Gibbs Measure for the Ising system is a hard task (except for the 1-dimensional case, for which the result is trivial). Nonetheless, the approximated Mean Field Theory give us the possibility of grasping its qualitative behaviour.

The Mean Field Approximation could be derived from the variational principle of minimal free energy, when restricted to some simple measures (i.e., factorized ones,  $\mathcal{Z}[\mathbf{z}] = \prod_i z_i(\sigma_i)$ ), which neglect correlations among spins.

For example, for the Ising Model, one can choose the single-spin measure to be such that the average magnetization is  $m$

$$m = \langle \sigma \rangle = \frac{\text{prob}(\sigma = +) - \text{prob}(\sigma = -)}{\text{prob}(\sigma = +) + \text{prob}(\sigma = -)} \quad (1.18)$$

then, self-consistently, one has that a spin experiences an effective magnetic field, being the sum of the external field  $h$ , and the average interaction from the  $2d$  neighbours,  $2dJm$ , which determines

$$m_{\text{mf}} = \tanh(2\beta Jd m_{\text{mf}} + \beta h). \quad (1.19)$$

It is also interesting to determine the partition function, highlighting the different roles of energy and entropy. The number of accessible configurations with average magnetization equal to  $m$  is given by a binomial coefficient, which, by Stirling expansion, gives

$$S(m) = \frac{N}{2} ((1 - m) \ln(1 - m) + (1 + m) \ln(1 + m)), \quad (1.20)$$

while the average energy is

$$E(m) = N (hm + dJm^2). \quad (1.21)$$

Figure 1.1 gives hints about the free energy landscape of the Ising Model with zero external field, parametrized by the mean magnetization. In particular the figure shows that for systems with temperatures under a critical point (The Curie Temperature,  $T_c$ ), the minimal free energy point is realized in two different “phases”, symmetrical w.r.t. inversion of all the spins. In other words, at  $h = 0$  in dimension  $d > 1$ \* Ising Model experiences a *Spontaneous Symmetry Breaking* (SSB), since the Hamiltonian function symmetry under the spin-flip transformation (with  $h = 0$ )

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\*note that MFT is too crude in the 1-dimensional case to derive such result that came by other techniques. Actually MFT could be seen as the zeroth order of approximation in a  $1/d$  expansion leading exact results in the  $d = \infty$  limit.

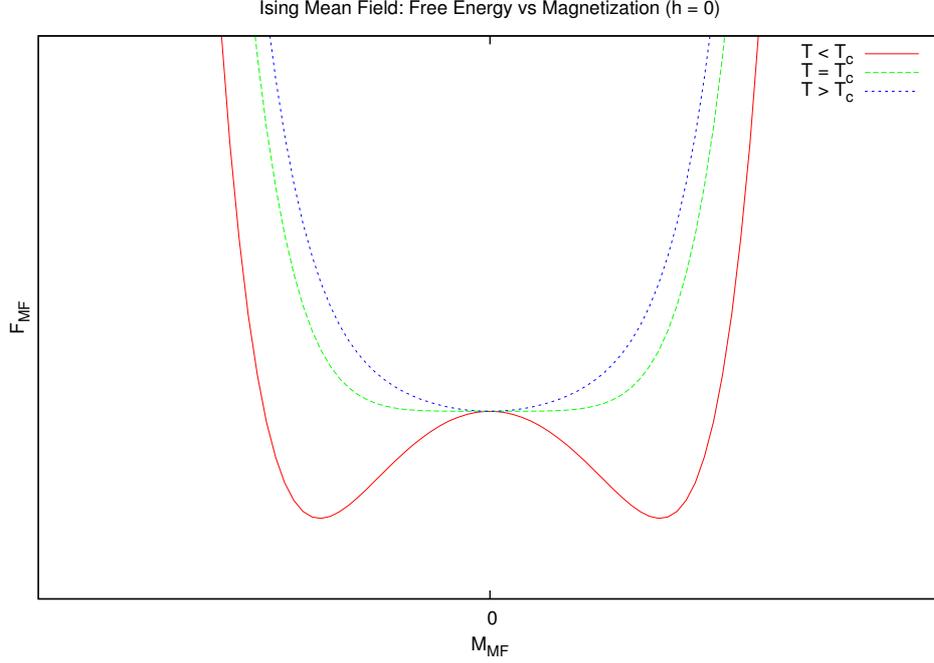


Figure 1.1: Qualitative picture of the Free Energy landscape in the MF Approximation with no external magnetic field for temperature at, above and below Curie Temperature  $T_c$ .

causing zero magnetization expectation at equilibrium, spontaneously\* fails to happen in sub-critical temperatures, due to the existence of two ergodicity basins for the dynamics, such that the system gets trapped in one of them (for an infinite time, in the thermodynamic limit).

At least in its dynamic aspects, the concept of *pure phase* is based on this ergodicity breaking<sup>†</sup>. For Ising Model, let us consider these two limit measures:

$$\mu_+^T(\boldsymbol{\sigma}) = \lim_{h \rightarrow 0^+} \mu_{\text{Gibbs}}^{(T,h)}(\boldsymbol{\sigma}) \quad \mu_-^T(\boldsymbol{\sigma}) = \lim_{h \rightarrow 0^-} \mu_{\text{Gibbs}}^{(T,h)}(\boldsymbol{\sigma}) \quad (1.22)$$

They clearly do not coincide because of  $\langle m(\boldsymbol{\sigma}) \rangle_+ = -\langle m(\boldsymbol{\sigma}) \rangle_- > 0$  (it even tends to 1 as  $T \rightarrow 0$ ), and, on the critical line ( $h = 0$ ,  $T \in [0, T_c]$ ) in the parameter space  $(h, T)$ , the Gibbs measure, as well as any equilibrium measure allowed in the system, are a convex combination of them, and we say that there is *phase coexistence*, like, for example, in a closed container at  $100^\circ$  and density intermediate between  $0.001\text{g/cm}^3$  and  $1\text{g/cm}^3$ , there is coexistence of water and vapour (see for example (1.3))

$$\mu_{(\lambda)}^T(\boldsymbol{\sigma}) = \lambda \mu_+^T(\boldsymbol{\sigma}) + (1 - \lambda) \mu_-^T(\boldsymbol{\sigma}) \quad \lambda \in [0, 1]; \quad \mu_{(\text{Gibbs})}^T(\boldsymbol{\sigma}) = \mu_{(\lambda=1/2)}^T(\boldsymbol{\sigma}) \quad (1.23)$$

\*as opposed to an explicit breaking via  $h \neq 0$ .

<sup>†</sup>with which also the uniqueness of the equilibrium measure fails.

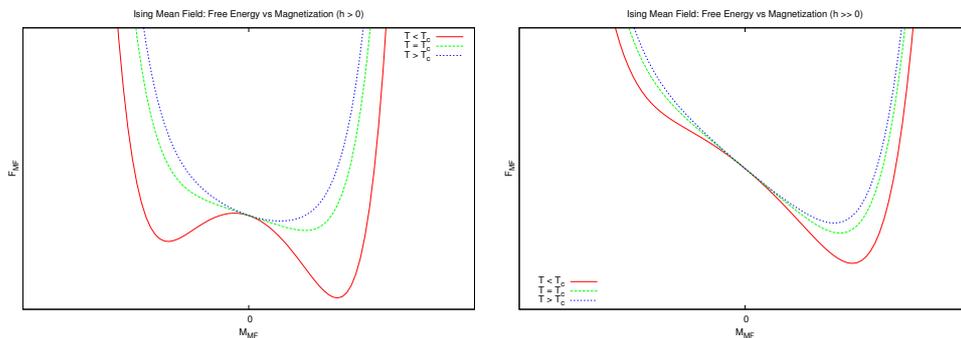


Figure 1.2: Qualitative picture of the Free Energy landscape in the MF Approximation with positive external magnetic field for temperatures at, above and below Curie Temperature  $T_C$ .

It turns out that, when the SSB occurs, one has an analytic signature of this phenomenon in the expression for the free energy. Indeed, at finite size the partition function is an integral of a positive regular function (or a positive-coefficient polynomial in algebraic variables, as in the case of discrete variables, e.g., in a spin system), and thus it must be infinitely differentiable, as well as its logarithm. Nonetheless, our statement on the fact that the free energy is extensive is realized through a non-trivial mechanism: it just states that the limit  $\lim_{N \rightarrow \infty} \mathcal{F}(\beta, N)/N$  exists, but the limit of a sequence of differentiable functions could well be a non-differentiable one!

What happens is that the points in the phase space (e.g., in the plane  $(T, h)$ ) at which the free energy fails to be analytic are the natural candidates for the ones at which SSB occurs. This phenomenon is pictorially clear on our graphics for the mean-field Ising Model: what is continuous is the free energy functional calculated at the value  $m = 0$ , which is the one selected by the variational principle for  $T > T_C$ , as well as at any differentiable curve  $m = m(T)$  that one could choose to follow. But the SSB causes a “fork” of the symmetric minimum  $m = 0$  into the two minima  $m = \pm m^*$ , exchanged by the symmetry, thus the position of the minimum along  $T$  is not a differentiable function.

Finally we spend some more words on the concept of pure phases, and how to characterize them in those regions where there is coexistence of phases. As the “label” of the pure phase is some global quantity, it causes some common background for all the variables, being the effect of a local cooperative behaviour of the degrees of freedom in the system, which appears like breaking the locality condition (two variables, well separated in space and at the same time, know that they are in the same phase, even without sharing information through the propagators of the physical dynamics!). Clearly, there is no paradox in this, as our conclusions, which assumed thermalization and large-volume limit, imply that there is actually no information to “exchange”,

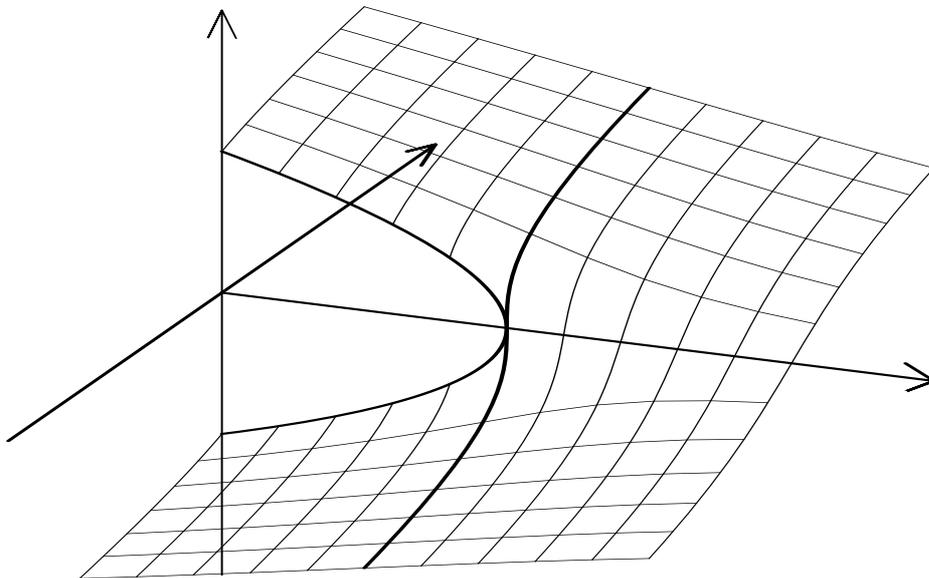


Figure 1.3: Qualitative picture of the Magnetization dependence on the parameters space.

because the phase label is fixed. Nonetheless, this apparent breaking of locality has a well-defined set of consequences on the set of physical observables in the system, and, turning things upside-down, it allows to determine a non-ambiguous analytical recipe for characterizing the “pure phases”, i.e., the phases which are not a non-trivial convex combination of other phases. This criterion comes under the name of *cluster property*:

**Cluster Property** Given an equilibrium measure  $\mu$ , it describes a pure phase if and only if, in the thermodynamic limit, given the local observables  $A_i(x)$  – where “locality” means that

$$\lim_{|x-x'|\rightarrow\infty} [A_i(x), A_i(x')] = 0 \quad (1.24)$$

$$\lim_{|x-x'|\rightarrow\infty} (\langle A_i(x)A_j(x') \rangle - \langle A_i(x) \rangle \langle A_j(x') \rangle) = 0 \quad (1.25)$$

### 1.3 Disordered Systems

Glassy systems are characterized by the presence of some sort of structural disorder in addition to the thermal one. They arise as result of a range of phenomena like impurities or the fast cooling of viscous materials which prevent from the formation of the crystal lattice.

Spin glass models try to reproduce this feature through a microscopic local fluctuation of the parameters in the Hamiltonian function, that thus now contains an extensive number of parameters, whose knowledge is only probabilistic (for example coming from the various distances of atomic positions in a glass). Standard treatments assume  $\mathcal{H}_{\mathbf{J}}(\mathbf{x})$  depending on these parameters, called *quenched* variables  $\mathbf{J} = \{J_1, J_2, \dots, J_k\}$  where  $k$  runs for example on the number of two-site interactions. They are called *quenched* variables because they arise typically throughout a concurrent process of different time scales, like in a freezing process where the system remains trapped in a metastable structure, while thermalization to equilibrium of other sets of variables is comparatively very rapid.

Magnetic systems are commonly considered with typical Hamiltonian functions like:

$$\mathcal{H}_{\mathbf{J}}(\boldsymbol{\sigma}) = \sum_{i,j} J_{ij} \sigma_i \sigma_j \quad (1.26)$$

where spin variables take value in  $\{\pm 1\}$ , while interaction parameters are random variables with some assumptions about the first moments of their distribution. The analytical treatment is rather difficult, so that simplifications are essential for deriving any results from these models. Nonetheless, our analysis of the Ising example shows that even a crude simplification could maintain some aspect of the desired original system. Different models arise when changing the distribution of the quenched variables or the underlying graph of interactions. Here is a list of models widely studied in the spin glasses literature for their interesting properties under the Mean Field Approximation:

**SK** The Sherrington-Kirkpatrick Model adopts a “normal” (i.e., Gaussian) distribution of the quenched random variables on every pair of spins. Variance is assumed to scale as  $1/\sqrt{N}$ , in order to have a good scaling of the extensive quantities, such as the internal energy. It is the random-interaction Ising system more “near” to the fully-connected system where, in the analogous fixed- $J$  Ising model, the mean-field approximation is exact, thus it was considered conceivably as the easiest disordered system to study. However, as it is well known, this model shows new and complex features, which can be understood at the light of the Parisi solution for the quenched free energy. In this context, the crucial concept of spontaneous Replica Symmetry Breaking is introduced [1].

**VB** The Viana-Bray Model or Bethe Lattice model has spin variables on a random lattice, where  $z$  is the mean coordination of the graph, finite in the  $N \rightarrow \infty$  limit. In this case, just  $Nz/2$  parameters are different from zero, and this is expected to reproduce some more “physical” situations, from condensed matter physics, where  $z$  is related to the volume of some short range interaction. Nonetheless, the fact that the graph is random still keeps some analogy with a mean field approximation, in the fact that, on a finite-dimensional

geometry, the “neighbour of a neighbour of a neighbour...” of a site has a higher chance of being a neighbour of that site, w.r.t. the average. The higher is the dimension, the smaller this effect is, up to disappear at  $d = \infty$ . But, as we said, this limit is another one in which the ferromagnetic Ising model was exactly described by the mean-field solution.

**EA** The Edwards-Anderson Model has pairwise interactions between nearest neighbours on a regular  $d$ -dimensional lattice, just like the Ising Model, but where coupling parameters are random variables. This is the most “physical” example, but of course an impossible challenge at high dimension ( $d \geq 3$ ), where not even the regular case is solved, while the  $d = 2$  case admits a spin-glass transition, if any, only at  $T = 0$  (analogously to regular Ising in  $d = 1$ ).

A recurrent phenomenon in these models is the *frustration*, i.e., the existence, in opposition to the ordered models like Ising, of interactions whose tendency on the system is towards antagonistic configurations. Frustration may emerge for example in the anti-ferromagnetic ( $J < 0$ ) Ising Model when it is applied to non bipartite lattices (where a chessboard-like disposition is not possible), such as a triangular lattice. However frustration can also arise easily on arbitrary “loopy” graphs, when the interactions  $J_{ij}$  are allowed to take values with different signs.

An extensive number of frustrated interactions is the microscopic root of the existence of a very rough free energy landscape for these models, where not only the number of pure phases could grow exponentially (with free energy shifts of order 1), but also it results very difficult to identify some *order parameter*, like the mean magnetization for Ising, capable of distinguish and label the pure phases in a simple way.

As standard thermodynamics is involved in the calculation of the free energy for deriving a set of macroscopic quantities from that, in the study of glassy systems it is very important the calculation of the so called *quenched averages*, as opposed to the usual and somewhat better-behaving *annealed averages*, defined as follows:

$$\langle A \rangle_{\text{quenched}} = \overline{A} = \int d\mu(\mathbf{J}) \langle A \rangle_{\mathbf{J}} \quad \text{with} \quad \langle A \rangle_{\mathbf{J}} = \frac{1}{\mathcal{Z}_{\mathbf{J}}} \int_X d\boldsymbol{\sigma} e^{-\beta \mathcal{H}_{\mathbf{J}}(\boldsymbol{\sigma})} A(\boldsymbol{\sigma}) \quad (1.27)$$

$$\langle A \rangle_{\text{annealed}} = \frac{1}{\overline{\mathcal{Z}}} \int_X d\boldsymbol{\sigma} \int d\mu(\mathbf{J}) e^{-\beta \mathcal{H}_{\mathbf{J}}(\boldsymbol{\sigma})} A(\boldsymbol{\sigma}) \quad (1.28)$$

It is relatively easier to deal with annealed averages, which provide a bound to the analogous quenched ones, although often a quite poor one, and, in the case of a critical phenomenon, they lack to show the same non-analyticities of the quenched homologous. Understanding this “two-level” averaging seems thus to be a crucial point.

A further intuition on this fact comes from the observation that thermodynamic averages could be almost independent from the realization of the disorder, on average and in the thermo-

dynamic limit – we say in this case that these quantities are *self-averaging*, i.e. for a quantity  $A$

$$\lim_{N \rightarrow \infty} \frac{\overline{(A - \langle A \rangle_{\mathbf{J}})^2}}{A^2} = 0 \quad (1.29)$$

while other quantities could fluctuate extensively with the size of the system – we say in this case that these quantities are *non-self-averaging*. For example, the free energy is a self-averaging quantity in all “well-behaving” models, but the Parisi parameter  $q(x)$  is not self-averaging in the SK model.

Random systems usually require a refinement of the Mean Field Approximation or, sometimes, new techniques such as the replica trick used to derive a solution for the SK Model. In particular, from the solution of this model very nontrivial conclusions were derived about the structure of the phase space. The Replica hierarchy was developed in order to get an overview of the many phases breaking and its ultrametric structure. “Easy” systems are the ones respecting the *Replica Symmetry* (RS) and they are characterized by the existence of a unique pure phase, while more complex cases exist ranging from the *1-step replica symmetry breaking* (or 1-RSB) to  $\infty$ -RSB, meaning for that the existence of graded levels of pure phases (called *clusters* of phases, and then *clusters of clusters* of phases, when pictorially speaking, etc.).

## Chapter 2

# Combinatorial Optimization

The purpose of this chapter is to introduce concepts and problems of Combinatorial Optimization, as this is the proper framework for discussing the Assignment Problem.

After that we will present the Hungarian Algorithm, a strongly polynomial algorithm for the Assignment Problem. Its interest is twofold: on the one hand it provides a meter of comparison for effective algorithms in this field, on the other hand its analysis introduces the dual problem related to the assignment, which clarifies some structural aspects of the problem, and will lead to the determination of an optimality certificate, also in our Cavity approach.

### 2.1 Combinatorial Optimization

Basic ingredients of a combinatorial optimization problem are (a) a set of input objects defining a particular instance to be solved, (b) a finite space of feasible solutions, typically exponentially large, and (c) a cost function over this space to be minimized or maximized.

For a precise mathematical representation of these problems it is often used the graph theory language. A graph  $G$  is defined by a set of points  $V$ , called nodes or vertices, and a set of edges  $E$  linking couples of them.

Here is a list of prototype problems:

**Shortest Path Problem** Find a minimal length path between two given nodes in a graph  $G$ .

**Travelling Salesman Problem** Find a minimal Hamiltonian path in a graph  $G$ , i.e., a tour passing through each node exactly once and returning to the starting point.

**Chinese Postman Problem** Find a minimal tour in a graph  $G$  passing through each edge at least once.

**Max Flow Problem** Given a *flow*  $F$ , i.e., a graph and a numerical function from its edges defining the “capacities”, find a maximal numerical function from the edges with values less than those of capacities, i.e., a maximal flow between a starting point (source) and a final one (sink).

**Chromatic Number Problem** Find the chromatic number of the graph  $G$ , i.e., the minimum number of colours sufficient to colour each node in such a way that no two adjacent vertices share the same colour.

All these problems share a finite space of feasible solutions so the emphasis is not too much about the standard questions in mathematics, like existence and uniqueness, but rather on the search and analysis of efficient recipes (algorithm) solving instances of these problems.

An algorithm is, loosely speaking, a procedure for solving a problem. More precisely it is a set of instructions understandable by an appropriate automatic machine, such that, given some input data in a finite number of steps leads to some output. Inputs are a representation of an instance of the problem claimed to be solved by the algorithm, as outputs are supposed related to the solution.

A formal definition of algorithm is rather subtle and it is investigated by Computability Theory via concepts of the Universal Turing Machine,  $\lambda$ -calculus, and the theory of formal languages (see for example [5]). Here it suffices to say that the *Church-Turing Thesis* is the fundamental hypothesis in Computation Theory stating roughly that all possible computation\* can be performed by an algorithm running on computers provided with an infinite amount of time and space.

However simple algorithms are known since the dawn of mathematics, like the Euclid algorithm for the computation of the GCD between two integers ( $\sim 300$  BC):

---

**Algorithm 1** Euclid’s algorithm

---

1: <b>procedure</b> EUCLID( $a, b$ )	$\triangleright$ The g.c.d. of $a$ and $b$ , with $a \geq b$
2: $r \leftarrow a \bmod b$	
3: <b>while</b> $r \neq 0$ <b>do</b>	$\triangleright$ We have the answer if $r$ is 0
4: $a \leftarrow b$	
5: $b \leftarrow r$	
6: $r \leftarrow a \bmod b$	
7: <b>end while</b>	
8: <b>return</b> $b$	$\triangleright$ The g.c.d. is $b$
9: <b>end procedure</b>	

---

\*There are, of course, examples of impossible computation like the *Halting Problem*, and others related to the Gödel theorems about incompleteness.

This simple example shows the basic features of the informal characterization of the algorithm concept:

1. a finite set of input data  $(a, b)$  to be properly encoded in order to make them “understandable” from the calculating matching,
2. a finite set of output data as  $b$  at line (8),
3. a number of steps during which the internal state of the calculating device is changed. This steps should be simple enough to be properly computed in an automatic way in a finite time by the underling calculator.

A feature to be remarked is that the number of steps necessary to complete the calculation is dependent on the input data, and, although in this case, the finiteness of the number of steps is beside any doubts, in general, it is not a simple question to determine if an algorithm will definitively stops on every possible input. Already in our easy example, the any case finiteness of the procedure is based on an elementary application of a subtle concept: the existence of a (strict) Lyapunov function, i.e., a function valued in  $\mathbb{N}$ , such that the initial value is finite, and in the given bounded-time procedure either the algorithm succeeds, or the value decreases by a finite amount. In this case, the value of variable  $a$  is a good Lyapunov function, w.r.t. the “while” loop.

Many features of the algorithm determine its efficiency, like storage required for the internal state of the computing machine. But usually people tends to focus on the number of steps required to complete the calculation. Given an algorithm  $\mathcal{A}$  adapt to run on a machine  $\mathcal{M}$ , we define the integer function  $f^{\mathcal{A}\mathcal{M}}(I)$  as the number of steps required to get the final answer from the input  $I$ , using the algorithm  $\mathcal{A}$  implemented on a machine  $\mathcal{M}$ . Even if its actual form is relatively of little interest, because of its widely variability with the implementation details, and also in the space of the input data, nonetheless theoretical enquire concentrates on its leading term in the scaling behaviour with a proper size function of the input data. For the Euclid’s algorithm a natural choice is the magnitude of the input numbers  $(a, b)$ , for other problems, like those reported at the beginning of the section, could be better using the size of the underling graph as the number of vertices and/or the number of edges.

In our Euclid case, for example, the time spent inside any of the “while” loop depends on how well is performed the integer division, but this is clearly a technical point of small relevance. What is important is that we can prove that the “while” loop is invoked a number of times bounded by some function of the input sizes  $a$  and  $b$ , namely, smaller than  $2 \log_2 a$  (indeed, after two steps one gets  $(a_t, b_t) \rightarrow (b_t, r_t) \rightarrow (r_t, \cdot) \dots$ , so that  $a_{t+2} = r_t$ : in the case  $b_t \geq a_t/2$  one gets  $a_{t+2} = r_t \leq a_t/2$ , while in the case  $b_t \leq a_t/2$  one gets  $a_{t+2} \leq a_{t+1} = b_t \leq a_t/2$  – this proves that  $a$ , and even  $\lfloor \log_2 a \rfloor$  if we group loops in pairs, are Lyapunov functions).

Theoretical treatment in Computer Science tends to concentrate on the *worst-case analysis*, as defined from:

$$\lim_{N \rightarrow \infty} \max_{|I|=N} f^{\mathcal{AM}}(I) \quad (2.1)$$

where the limit process just suggests our interest in the asymptotic behaviour.

Practical consideration may also be directed to some form of *average-case* analysis, which indeed is the principal case for many real-life application, and meets the tools inspired by physics, an more specifically by statistical mechanics:

$$\lim_{N \rightarrow \infty} \sum_{|I|=N} p(I) f^{\mathcal{AM}}(I) \quad (2.2)$$

where  $p(I)$  indicates a proper probability distribution in the input space.

As an example of the importance of implementations details of the underling machine, consider the problem of numbers encoding. Numbers enter in the calculation in a specific representation, even if the mathematical formalization can hide this point. Usually three kinds of encoding are discussed:

**unary encoding** when a natural number  $n$  contributes with  $n$  at the determination of the input size, i.e., when one represents numbers like 5 as IIIII.

**binary encoding** a binary representation of an integer  $n$  contributes with  $1 + \log_2[n]$  to the input size (5 is encoded as 101). This is the encoding of “real-life” machines.

**arithmetic encoding** in this case any integer number gives a single contribution to the input size.

It should be clear that really different behaviours emerge in the functions (2.1) and (2.2) with respect to different encoding paradigms. For example, our Euclid Algorithm is linear in binary encoding, but unbounded in arithmetic encoding, while also vice-versa could happen (algorithms could be e.g., polynomial in arithmetic encoding, and unbounded in binary encoding, cfr. for more details [3], box 2B).

The relevant concept of complexity of an algorithm is a bit subtle, as it involves in some convoluted way worst-case reasonings and large-size limits. In order to better describe the concept, it is useful to introduce in the asymptotic analysis the so-called “big oh” notation, defined as follows:

Given two functions  $f$  and  $g$ , from  $\mathbb{N}$  to  $\mathbb{N}$ , we say that  $f = \mathcal{O}(g)$  iff there exists constants  $c$  and  $n_0$  such that, for all  $n \geq n_0$ ,  $f(n) \leq c g(n)$ .

Big oh notation naturally create an order structure in the scaling aspects of the algorithms: an equivalence relation is defined as  $f = \mathcal{O}(g) \wedge g = \mathcal{O}(f)$  saying that  $f$  and  $g$  has the same *rate*

of growth ( $f \asymp g$ ), and between equivalence classes of rate of growth is defined a partial order relation as  $f \preceq g$  if  $f = \mathcal{O}(g)$ .

## 2.2 Complexity Classes

Thanks to the big oh notation and the related partial order relation it is possible to classify algorithm in complexity classes. We say that an algorithm  $\mathcal{A}$  belongs to  $\text{TIME}(f)$  if

$$\max_{|I|=N} f^{\mathcal{A}}(I) = \mathcal{O}(f(N)) \quad (2.3)$$

This in turn leads to a classification for the problem itself, supposed to be solved by the algorithm  $\mathcal{A}$ , through:

$$\min_{\mathcal{A} \text{ solving } P} \max_{|I|=N} f^{\mathcal{A}}(I) = \mathcal{O}(f(N)) \quad (2.4)$$

Complexity classes can then classify the subset of problems called *decision problems*, i.e., problems whose solution is just a binary information like true or false. In this subclass, the analysis is simplified, because there is a simple formulation in terms of formal languages. This is not the case in general for the more familiar *function problems*, i.e., those whose solution is a more complex output like a number, or a graphical structure.

For the moment let us observe that it's easy to derive natural decision problems from a function problem, and also, that this distinction is weaker than it could look. For example, in many cases a function problem could be easily decomposed into a set of decision problems. Consider the problem of finding the set of boolean variables  $x = (x_1, \dots, x_n)$  such that the cost function  $C(x) : \{0, 1\}^n \rightarrow \{0, \dots, 2^m - 1\}$  is minimized. Then, one could consider the decision problem such that, for a value  $a$  and a subset of fixed conditions  $(S, y)$ , with  $S \subset \{1, \dots, n\}$  and  $y = \{y_j\}_{j \in S}$ , asks whether there exists an assignment  $x$  such that  $x_j = y_j$  if  $j \in S$ , and  $C(x) \leq a$ . Then, by Newton method on  $a$ , one can determine the value of the minimum cost in at most  $m$  steps, while fixing recursively the variables one can also find a realization of  $x$  in at most other  $n$  steps.

Furthermore, even inside the classes of decision or function problems (and for other classes), there exists a relevant concept of “equivalence for what concerns the complexity” (up to some factor), which goes under the name of *reduction*. Say that, for two problems  $\mathcal{P}$  and  $\mathcal{P}'$ , there exists a way of formulating a whatever instance of the first one, of size  $n$ , as an instance of the latter, of size  $\sim n^a$ , in the sense that, if we could solve the new instance, we would implicitly solve the original problem. Then, clearly, if we could prove that second problem is, say, of polynomial complexity with degree  $c$  (i.e., times scale as  $n^c$  in worst case), then the complexity of the original problem could not be larger than polynomial of degree  $ac$ . In particular, if  $a = 1$  we would have a *linear reduction*, so that, if  $\mathcal{P}$  can be reduced to  $\mathcal{P}'$  and vice-versa, the two problems have the

same complexity, while in the most common case in which  $a$  is finite, although not necessarily 1 (*polynomial-time reduction*), we would have that the first problem can not be “worse than polynomial” if the first one is polynomial.

An example of linear reduction is the reduction of Assignment Problem to a case of Min-cost–Max-flow Problem on a specially structured graph (namely, a complete bipartite graph, plus one source and one sink, attached respectively to the left- and right-vertices, and all unitary capacities, cfr. section 2.3). Indeed, in this case, the fact that the Edmonds-Karp algorithm could solve an instance of Min-cost–Max-flow in polynomial time is already a proof of the fact that Assignment is polynomial, although the specially-devised Hungarian Algorithm (actually in part a specialization of the Edmonds-Karp ideas) has slightly better performances.

A look at the problems listed at the beginning of the chapter shows that a poor implementation of a searching procedure leads immediately to impractical solving times. The reason for this lies in the size of the space of feasible solutions, generally exponential in  $n$ , if not of order  $n!$  (which is even worse). This fact suggests that an exponential growth of solving time in dependence of the input size is the hallmark of intractable problems. On the other hand the set of problems with the hope of a “practical solution” should behaves with a polynomial rate growth in the size of the input.

The fact that implementation details can give to an algorithm a slightly better or worse performance, and the fact that the common procedure of polynomial reduction “bridges” problems in different-degree polynomial classes, suggests that one could separate in a qualitative sense the class of tractable and intractable problems, where the first ones are polynomial ones, regardless from their degree. So we have the classes

**P:** Polynomial time decision problems are defined as

$$P = \bigcup_{k \in \mathbb{N}} \text{TIME}(n^k) \quad (2.5)$$

and they form the class of problems that, in our assumptions, have some practical solving algorithm.

**EXP:** Exponential time decision problems are defined as

$$\text{EXP} = \bigcup_{k \in \mathbb{N}} \text{TIME}(2^{n^k}) \quad (2.6)$$

and they form the class of problems that, in our assumptions, are lacking of a practical solving algorithm.

In particular, a “loop” of polynomial reduction among  $k$  problems, and a proof that one of them is in  $P$ , automatically proves that all of them are in  $P$ , and similarly for  $\text{EXP}$ .

Their relation is easily seen as a proper inclusion:  $P \subsetneq EXP$  because there are many examples of problems that genuinely live in  $EXP$ .

There are, however, many problems whose complexity does not seem inherently non-polynomial, even if no polynomial algorithm is found for solving that problems. Besides a few exceptions (such as graph isomorphism), most of them are in a class that we define below, called  $NP$ . This motivates us to recall the concept of *Non-deterministic Turing Machine*. The modelization of an automatic calculating device is done by an Universal Turing Machine capable of changing its internal status step by step with a functional relation with the input data and the current state. The non-deterministic Turing machine is a conceptual machine capable of a non-functional evolution, maintaining at a generic step multiple copies of its internal state, and evolving them in parallel. In other words, a Non-deterministic Turing Machine is one with the capacity of branching its process at no cost.

This feature creates a parallel hierarchy to that built upon  $TIME(f)$ , where the basic class is replaced by  $NTIME(f)$ , that is the class of algorithm (or indirectly problems) such that, in a framework of non-deterministic machine, the rate of growth of time with the input size  $n$  is not greater than  $f(n)^*$ . In particular, all the reasonings about reduction translate immediately to these classes (as, in translation, are just applied “in parallel” to the branched processes). We have thus  $NP$  and  $NEXP$  analogously to  $P$  and  $EXP$  discussed above, and still one can prove, not only that  $NP \subsetneq NEXP$ , but even that  $NP \subseteq EXP$ . Remark however the sequence of inclusions

$$P \subseteq NP \subseteq EXP \subseteq NEXP \tag{2.7}$$

of which we do not know if any of the inclusion is strict ( $\subsetneq$ ) or instead an equality. The first question, in particular, whether  $P \subsetneq NP$ , is of quite large interest, as, through the strong concept of polynomial reduction, the class  $NP$  results to be populated by a huge number of relevant common-life problems (if you are curious, for the problems described at the beginning of the chapter, the shortest path, Chinese postman and max flow problems are known to be polynomial (and an algorithm is known for each), while the travelling salesman and the chromatic number problem are in  $NP$ ).

An insight of the  $NP \subseteq EXP$  inclusion comes from the pictorial intuition of the nondeterministic machine through the branched processes: we know that the depth of the resulting “tree of the processes” is polynomial, with some degree  $k$ , still we assume that every branching is finite, so that, w.r.t. the depth of the tree, the full size is at most exponential, with a finite rate (e.g.,  $2^{\text{depth}}$ ). Then, as a result, the whole complexity on the deterministic machine, which is forced to explore each branch in sequence, is bounded by the size of the tree, which is bounded by  $2^{n^k}$ , and thus is in  $EXP$ .

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\*For this sometime  $TIME(f)$  is replaced by  $DTIME(f)$ , for stress the deterministic feature of this class.

The complexity class NP aims to capture the set of problems whose solutions can be efficiently *verified*. The famous P vs NP question asks whether or not the two are the same. The resolution of this conjecture will be of great practical, scientific and philosophical interest. So, apart from the non deterministic Turing Machine, it is possible to fully characterize NP as the class of problems for which *succinct certificates* exist: appreciate a Beethoven sonata is far easier than composing the sonata, verifying the proof of a theorem is easier than coming up with a proof itself, and so forth. The P vs NP question thus asks whether exhaustive search can be avoided in general.

Informally speaking P is the class of all sets  $L$  such that the membership of an element  $x$  in  $L$  can be tested efficiently. On the other hand, NP is the class of all sets  $M$  such that every element  $y$  in  $M$  has a succinct certificate  $z$  that establishes the membership of  $y$  in  $M$ . Consider for example the set  $C \subset \mathbb{N}$  of composite numbers. There is no clear way to test efficiently whether a number, say 4,294,967,297 is composite. However, every number in  $C$  does have a succinct certificate, such as 6,700,417 and 641 whose product gives exactly 4,294,967,297. But finding it may be extremely hard\*.

## 2.3 The Hungarian Algorithm

The linear Assignment Problem is an optimization problem consisting in finding, given a  $n \times n$  matrix  $W = \{w_{ij}\}$ , with values in some numerical set<sup>†</sup>, a subset of elements in  $W$ , with exactly one element in each row and in each column<sup>‡</sup>, for which their sum is minimal.

$$W \in M_{n,n}[\mathbb{X}] \quad \text{find } \pi^* \in \mathfrak{S}_n \quad \text{such that}$$

$$\pi^* = \min_{\pi \in \mathfrak{S}_n} \sum_{i=1}^n w_{i\pi_i} \quad (2.8)$$

A graphical representation consists in a complete bipartite graph  $G = (S, T)$  with  $|S| = |T| = n$ , over whose edges is defined a cost function  $w : S \times T \rightarrow \mathbb{X}$ . The solution is the matching  $M$  with minimal cost defined as:

$$\text{cost}(M) = \sum_{e \in M} w(e) \quad (2.9)$$

As the space of perfect matchings in a complete bigraph is  $n!$ , defining the space of feasible solution a naïve search leads to a non polynomial time ( $\mathcal{O}(n!)$ ), nevertheless strongly polynomial algorithms are found capable to identify a solution in  $\mathcal{O}(n^3)$ .

---

\*The above factorization was first discovered by the mathematician Leonard Euler in 1732, a full 92 years after Fermat had conjectured that no such factorization existed.

<sup>†</sup>First studies focused on integers, or rational values, but also the real case hides some remarkable features.

<sup>‡</sup>i.e., a permutation of  $n$  elements  $\pi \in \mathfrak{S}_n$ .

Here we want to present a very effective (actually  $\mathcal{O}(n^3)^*$ ) and classical<sup>†</sup> algorithm for the Assignment Problem. The algorithm dates back in an article of Harold Kuhn in 1955 ([6]), and was called Hungarian as a tribute for the two main results on which is based, discovered since the 1930s by two Hungarian mathematicians, Kőnig and Egerváry.

Kőnig theorem focuses on a characterization of bigraph with a perfect matching. Better, as explained by Lovász, he discover a *well-characterization*, meaning for this, a NP-property whose negation is also an NP-property<sup>‡</sup> (for an insightful exposition of this concept see box 1A in [3]), this *per se* does not give rise to a polynomial algorithm for finding a maximum matching in a bipartite graph. But its relevance is in the constructive way with which he demonstrates the theorem. In particular he introduces the fundamental concept of *alternating* path, which plays a central role in a plethora of combinatorial results.

Before of stating it let's remark a few of graph terminology: given a graph  $G = (V, E)$ , the points  $i$  and  $j$  are said adjacent if exists an edge  $e \in E$  joining them (in this case we can use  $e = (ij)$ ); two lines which share a point are also said to be adjacent. A graph in which every pair of nodes are adjacent is said to be complete. A set of lines in  $G$  is a matching if no two lines have a point in common. The size of any largest matching in  $G$  is called the matching number of  $G$ . If  $M$  is a matching of  $G$ , any point  $i$  in the graph is either matched, if some line exists in  $M$  that is incident with  $i$ , or exposed if no line incident with  $i$  exists in  $M$ . A set of points  $S \subset V(G)$  is a point cover of  $G$  if each line in  $E(G)$  has at least one endpoint in  $S$ . The cardinality of any smallest point cover is the point covering of  $G$ . Finally, we indicates with  $\Gamma(S)$  the set of points adjacent with any node in  $S$ .

**Theorem 1 (Kőnig 1916)** *If the graph  $G$  is bipartite, then the matching number  $\nu(G)$  equals the point covering number  $\tau(G)$ :*

$$\tau(G) = \nu(G) \tag{2.10}$$

Before to sketch the proof let's formulate it in a other way that remarks its minimax aspect<sup>§</sup>:

**Theorem 2** *Given a bipartite graph  $G = (S, T; E)$ , the minimum number  $\mu(M)$  of exposed elements of  $S$  by a matching  $M$  is equal to the maximum of the deficit number  $h(X) = |X| - |\Gamma(X)|$  of a set  $X \subset S$ :*

$$\min_M \mu(M) = \max_X h(X) \tag{2.11}$$

*In particular, a perfect matching is possible if and only if  $|\Gamma(X)| \geq |X|$  for all  $X \subset S$ .*

---

\*This scaling is really close to the fastest known algorithms for solving AP.

†As folklorist note, it celebrated its 50th birthday in 2005

‡i.e., it is in  $\text{NP} \cap \text{coNP}$ , being  $\text{coNP}$  the class of decision problems that ask for the non-membership of an elements in a NP-class problem. It could be surprising, but actually an active area of research is involved in determining whether these classes indeed coincided.

§see [3] for an explanation of the relevance of *minimax* theorems.

The constructive proof runs as follows: given a matching  $M$  consider  $S'$  and  $T'$ , the sets of exposed nodes in  $S$  and  $T$  by  $M$ . Build a *Hungarian Forest*  $Z$  with the following requirements: (1) every node in  $T$  has degree 2 and is incident with a matching edge, (2) each component in  $Z$  contains a point of  $S'$ . Pictorially it could be done superposing arrows on the edges in  $M$  toward  $S$ , and on the edges out of the matching toward  $T$ , then the Hungarian Forest is composed by any edge reachable through a directed path from a point in  $S'$ . By construction any path in  $Z$  is  $M$ -alternating, i.e., it alternates edges in  $M$  and those in  $E \setminus M$ . Now if  $V(Z) \cap T' \neq \emptyset$  we can improve the matching taking any of the alternating paths connecting  $S'$  and  $T'$  and reversing the matching membership in the alternating path (such a path is called for obvious reasons *augmenting path*). Otherwise if  $Z \cap T' = \emptyset$ , then  $L := (T \cap V(Z)) \cup (S - V(Z))$  is a set of nodes covering all edges and  $|M| = |L|$ . In particular the set of maximum deficiency is  $V(Z) \cap S$ .  $\square$

The idea of augmenting path presented in the proof can be easily applied for a maximum matching algorithm for bigraph:

---

**Algorithm 2** Algorithm for Maximum Matching in a Bigraph

---

```

1: procedure KÖNIG( $S, T, E, M$ ) ▷  $M$  could be  $\emptyset$ 
2:    $S' \leftarrow S - V(M), Z \leftarrow \emptyset$ 
3:   for all  $i \in S'$  do
4:     build a Hungarian Forest  $Z$  ▷ BFS or DFS can be used
5:     if alt-path  $A_i \subset Z$  terminates in  $T'$  then
6:       Reverse  $M$ -membership of edges in  $A_i$  ▷  $M$  grows by 1
7:       goto (2)
8:     else
9:       add  $A_i$  to  $Z$ 
10:    end if
11:  end for
12:  return  $M$  and  $Z$  as Hungarian Forest
13: end procedure

```

---

Egerváry theorems, instead, uses the Kőnig's results in weighted bigraph (over which is defined the Assignment Problem, and its converse the Maximum Weighted Matching Problem). The core of his discovery lies in the concept of *covering*, that is a succinct certificate of maximality for a matching. Let's state it:

**Theorem 3 (Egerváry 1931)** *Given a complete bipartite graph  $G = (S, T; E)$  with  $|S| = |T|$ , and an integer non-negative weight function  $w : E \rightarrow \mathbb{Z}_+$ , let's call a weighted covering of  $G$ , a*

function  $c$  from the set of nodes of  $G$  with non-negative integer values such that:

$$c : S \times T \rightarrow \mathbb{Z}_+ \quad \text{with} \quad c(i) + c(j) \geq w(ij) \quad \forall (ij) \in E, \quad (2.12)$$

Then the maximum weight of a perfect matching  $M$  is equal to the minimum weight of a covering  $c$ . In formulae:

$$\text{cost}(M) = \sum_{e \in M} w(e); \quad \text{cost}(c) = \sum_{v \in S \cup T} c(v); \quad \min_c \text{cost}(c) = \max_M \text{cost}(M). \quad (2.13)$$

Assuming for the proof that  $c$  is a minimal weight covering of  $G$ . Consider then the set of *tight* edges, defined as those for which holds  $c(j) + c(i) = w(ij)$ , and the subgraph  $G_c$  of tight edges. If a perfect matching in  $G_c$  exists, it is also a matching for  $G$ , and its weight is clearly minimal. Suppose else, that no such a perfect matching exists. Then König's theorem guarantees the existence of a deficiency set  $X \subset S$  such that  $|\Gamma_{G_c}(X)| > |X|$ , this in turn, allows us an improvement of the covering  $c$ : let's  $c'$  equals to  $c$  for all nodes, but those in  $X \cup \Gamma_{G_c}(X)$ , where it takes the values of  $c$  incremented by 1 over  $X$ , and decremented by 1 over  $\Gamma_{G_c}$ . If such function  $c'$  is not a covering, because of the possibility of  $-1$  values in  $T$ , then increment by one all values of  $c'|_{\Gamma_{G_c}(X)}$  and decrement all those in  $c'|_X$ . At this time we have a new covering  $c'$  with weight smaller than  $c$  resulting in a contradiction with the minimality assumption for  $c$ .  $\square$

The MWM algorithm resulting from the Egerváry theorem, easily extended to rational numbers, is nonetheless only *quasi-polynomial*, even if it used maximum deficiency set throughout the improvement procedure of recovering. The class of quasi-polynomial, as opposed to *strongly-polynomial*, time is related to the subtleties of information encoding

A strongly polynomial-time algorithm is one whose running time is bounded polynomially by a function only of the inherent dimensions of the problem and independent of the sizes of the numerical data. A pseudo-polynomial-time algorithm is one that runs in time polynomial in the dimension of the problem and the magnitudes of the data involved (provided these are given as integers), rather than the base-two logarithms of their magnitudes. Such algorithms are technically exponential functions of their input size and are therefore not considered polynomial. However, as Garey and Johnson (1979) observe, A pseudo-polynomial-time algorithm will display 'exponential behaviour' only when confronted with instances containing 'exponentially large' numbers.

The situation is analogous to the well-known case of maximum flow: for integer or rational capacities, the max-flow algorithm of Ford-Fulkerson\* (1956, [9]) is finite, but not strongly-polynomial, while with real capacities examples exists for which the algorithm is not even finite. The solving time actually depends on the size (magnitude) in value of the capacities. Nevertheless

---

\*which uses a strictly related concept to that of augmenting paths, i.e., *augmenting flows*.

---

**Algorithm 3** Algorithm for Maximum Weight Matching in a Bigraph

---

```
1: procedure EGERVÁRY( $S, T, w, c$ ) ▷ covering  $c$  could be trivial
2:    $E \leftarrow \emptyset$ 
3:   for all  $(ij) \in S \times T$  do
4:     if  $w(ij) = c(i) + c(j)$  then
5:       add  $(ij)$  in  $E$ 
6:     end if
7:   end for ▷ Here I have  $G_c$  of tight edges
8:   Compute  $M$  with KÖNIG( $S, T, E, \emptyset$ )
9:   if  $|M| = |S|$  then
10:    return  $M$  as MWM with covering  $c$ 
11:  else
12:    find  $X \subset G_c : |X| < |\Gamma_{G_c}(X)|$ 
13:    find  $d = \min\{c(j) + c(i) - w(ij) : u \in X, v \in \Gamma_G(X)\}$ 
14:    for all  $v \in S \times T$  do
15:      case  $v \in X : c'(i) \leftarrow c(i) + d$ 
16:      case  $v \in \Gamma_G(X) : c'(i) \leftarrow c(i) - d$ 
17:      case otherwise :  $c'(i) \leftarrow c(i)$ 
18:    end for
19:     $c \leftarrow c'$ 
20:    goto (2)
21:  end if
22: end procedure
```

---

Dinic (1970, [10]), and independently Edmonds-Karp (1972, [44]) proved that with a specific recipe (*Breadth First Search* for Edmonds-Karp) for selecting the augmenting flows, the Ford-Fulkerson algorithm can be transformed in a strongly-polynomial one.

In the case of Assignment (or MWM) the works of Harold Kuhn ([6]) fills the gap:

---

**Algorithm 4** Algorithm for Maximum Weight Matching in a Bigraph (*Hungarian Algorithm*)

---

```

1: procedure KUHN( $S, T, w, c$ ) ▷ covering  $c$  could be trivial
2:    $E \leftarrow \emptyset$ 
3:   for all  $(ij) \in S \times T$  do
4:     if  $w(ij) = c(i) + c(j)$  then
5:       add  $(ij)$  in  $E$ 
6:     end if
7:   end for ▷ Here I have  $G_c$  of tight edges
8:   Compute  $M, Z$  with KÖNIG( $S, T, E, \emptyset$ )
9:   if  $|M| = |S|$  then
10:    return  $M$  as MWM with covering  $c$ 
11:  else
12:    find  $d = \min\{c(j) + c(i) - w(ij) : u \in Z \cap S, v \in T - Z\}$ 
13:    for all  $v \in S \times T$  do
14:      case  $v \in T \cap Z : c'(i) \leftarrow c(i) + d$ 
15:      case  $v \in S \cap Z : c'(i) \leftarrow c(i) - d$ 
16:      case otherwise :  $c'(i) \leftarrow c(i)$ 
17:    end for
18:     $c \leftarrow c'$ 
19:    goto (2)
20:  end if
21: end procedure

```

---

A close look could observe that the main feature here is the integration of two separated parts of the Egerváry Theorem: computing the deficiency set and revising the covering. The Hungarian Algorithm could easily checked to be strongly polynomial:

1. there are at most  $|S|$  augmentation,
2. being the sets of nodes reachable from  $S'$  in  $G_c$  properly included in those reachable in  $G_{c'}$ , after at most  $|S|$  recovering an augmentation must happen,
3. the BFS (Breadth-First-Search) of nodes needs  $\mathcal{O}(|E|)$  steps, then the overall bound is  $\mathcal{O}(|E||S|^2) = \mathcal{O}(n^4)$ .

As it should be clear from the above exposition, the works of König, Egerváry and Kuhn face three aspects of the algorithm, namely:

1. König idea of alternating path provides a “local” transformation in the matching space, such that starting from any matching  $M$ , it gives rise to larger and larger matching in a polynomial number of steps.
2. Egerváry’s covering definition translate the weighted problem into a dual problem, allowing a reduction from the problem in the complete bipartite graph, to many unweighted problems in a not complete subgraph. This is possible thanks to the fact that the cover is a *certificate* of maximal weight of matching in the subgraph of tight edges.
3. Kuhn finally addresses the subtle question of the possibility of a big numbers of improvements in the Egerváry’s “gradient” driven algorithm. Physically may be thought as an improvement in selecting the steepest descent step, granting a strong polynomial bound in the number of steps.

Our implementation follows also the Munkres techniques [7] for speeding up the recovering procedure, as reported in Knuth [8], thus reducing the bound in  $\mathcal{O}(n^3)$ . Over random instances we derived the data presented in figure 2.1.

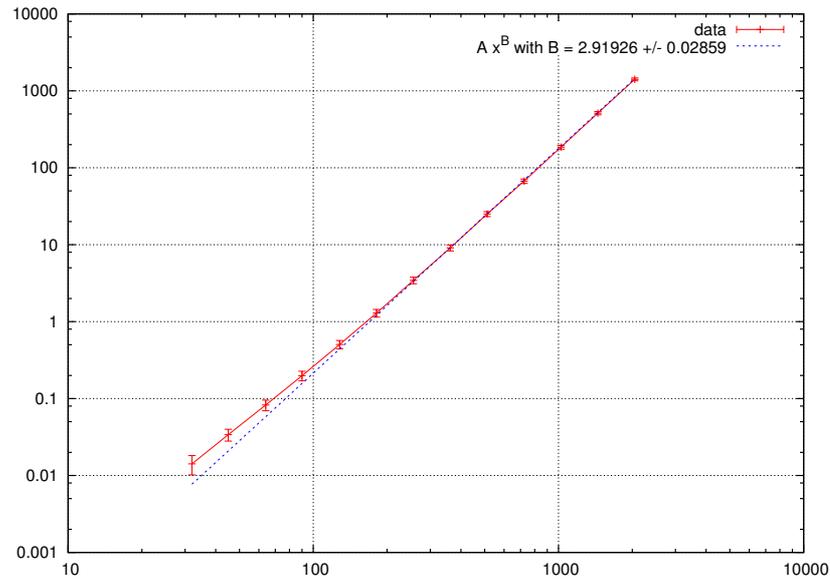


Figure 2.1: Plot of average solution times in an algorithmic implementation of the Hungarian Algorithm, applied to random instances in the ensemble described in the body of the chapter. One can evince that the average-case complexity is analogous to the worst-case discussed estimate, i.e., cubic in the size of the matrix. The algorithm follows the Knuth implementation (the source codes can be found in the literature), so this should assure you that, in comparing the performances of Cavity-inspired algorithms to the pre-existent Hungarian, we did not “cheat” by implementing the latter in a sub-optimal way!



## Chapter 3

# Cavity Theory for the Assignment Problem

In this chapter we introduce the Cavity Method, first through the Bethe Approximation for the Ising Model, then in a more general framework to fit the problems with randomness, and more generic forms of interaction. The method is developed only in the so-called *Replica Symmetric* (RS) assumptions, relevant to our case, while the *1-step Replica Symmetry Breaking* equations are not discussed, as pertinent to other classes of problems.

In the second part, we concentrate on the Assignment Problem. We describe the corresponding statistical mechanics model, and we specialize the cavity equations following the general treatment.

Finally, we add a few remarks on the goodness of the cavity approximation for our problem, both w.r.t. corrections of finite size, and to the stability of the assumption of the replica symmetry.

### 3.1 Bethe Approximation for Ising

The Bethe approximation is a refinement of mean-field theory, that neglects correlations coming from loops in the interactions graph.

Now we recall mean field equation for Ising in order to stress the similarity with the Bethe refinement. For a subset of sites  $A = (i_1, \dots, i_k)$ , we define the marginal probabilities  $p_A(\sigma_{i_1}, \dots, \sigma_{i_k})$  of the variables  $\sigma$  at sites in  $A$  (but, for short, we will often denote  $p_i(\sigma) \equiv p_{\{i\}}(\sigma)$ ).

$$p_i(\sigma) = \frac{1}{Z} \sum_{\sigma_j: j \neq i} \exp(-\beta \mathcal{H}(\boldsymbol{\sigma} | \sigma_i = \sigma)) \propto \sum_{j \in \partial i} p_{\partial i}^{(i)}(\sigma_{\partial i}) \exp(-\beta J \sum_{j \in \partial i} \sigma_j \sigma - h \beta \sigma) \quad (3.1)$$

where we used  $\partial i$  as the set of indices nearest neighbour of  $i$ , while the superscript  $(i)$  indicates a system in which interaction involving the variable at site  $i$  are removed. So  $p_{\partial i}^{(i)}(\sigma_{\partial i})$  indicates

the joint marginal probability of the variables  $\{\sigma_j\}$  for  $j$  in  $\partial i$ , in a system in which the factors containing  $\sigma_i$  in the Hamiltonian are deleted (indeed in the expression (3.1) are explicitly expressed apart) or, in other words, in a system in which a cavity is formed removing site  $i$ .

In order to get an equation for the mean magnetization, is thus necessary compute  $p_{\partial i}^{(i)}(\sigma_{\partial i})$ , and mean-field approximation assumes a simple factorized form for that (which actually neglects correlations):

$$p(\boldsymbol{\sigma}) \stackrel{\text{MF}}{=} \prod_j p_j(\sigma_j) \Rightarrow p_{\partial i}(\sigma_{\partial i}) \stackrel{\text{MF}}{=} \prod_{j \in \partial i} p_j(\sigma_j) \quad (3.2)$$

This, in turn, together with the translational invariance of Ising, yields an expression for the mean magnetization in a transcendental equation:

$$m = \tanh(\beta J z m + \beta h) \quad (3.3)$$

where we used  $z = |\partial i|$  as the connectivity of node  $i$  (that in general  $d$ -dimension squared lattice is equal to  $2d$ ).

Not surprisingly this approximation is rather crude in low dimensional model. For example the critical temperature in the case  $h = 0$  and in dimension 1, leads to  $\beta_c = 1/J$ , that is a quite disturbing result, provided that in the exact treatment  $\beta_c$  should be  $\infty$ . Of course for dimension higher and higher the approximation improves, until reaching the correct result in the  $\infty$ -dimensional case.

Bethe approximation starts with a somewhat smaller ‘‘cavity’’, that where a single link is removed: a system in which a single interaction is switched off having the Hamiltonian as

$$\mathcal{H}^{(i,j)}(\boldsymbol{\sigma}) = \mathcal{H}(\boldsymbol{\sigma}) + J\sigma_i\sigma_j = -J \sum_{\substack{\langle k,l \rangle \\ (k,l) \neq (i,j)}} \sigma_k\sigma_l - h \sum_k \sigma_k \quad (3.4)$$

We can write the marginal probability of the two variables for which their ‘‘inference channel’’ is interrupted:

$$p^{(ij)}(\sigma_i, \sigma_j) \propto \sum_{\sigma_{\partial j \setminus i}} p_{\partial j}^{(j)}(\sigma_{\partial j}) \exp \left\{ \beta h \sigma_j + \beta J \sum_{l \in \partial j \setminus i} \sigma_j \sigma_l \right\} \quad (3.5)$$

$$\propto \sum_{\sigma_{\partial i \setminus j}} p_{\partial i}^{(i)}(\sigma_{\partial i}) \exp \left\{ \beta h \sigma_i + \beta J \sum_{l \in \partial i \setminus j} \sigma_i \sigma_l \right\} \quad (3.6)$$

where the two choices (3.5) and (3.6) differ in which variable among  $\sigma_i$  and  $\sigma_j$  has been marginalized first (let’s name them for a moment ‘‘ $p_{j;i}^{(ij)}(\sigma_i, \sigma_j)$ ’’ and ‘‘ $p_{i;j}^{(ij)}(\sigma_i, \sigma_j)$ ’’ respectively). Calculating, for example, the magnetization on site  $i$  in the two frameworks leads to a consistency requirement

$$\langle \sigma_i \rangle = \sum_{\sigma_i, \sigma_j = \pm 1} \sigma_i p_{j;i}^{(ij)}(\sigma_i, \sigma_j) = \sum_{\sigma_i, \sigma_j = \pm 1} \sigma_i p_{i;j}^{(ij)}(\sigma_i, \sigma_j) \quad (3.7)$$

which leads to a relation among marginal probabilities  $p_{\partial j}^{(j)}(\sigma_{\partial j})$  and  $p_{\partial i}^{(i)}(\sigma_{\partial i})$ .

However, these relations are not sufficient to constrain in a self-consistent way the various relevant marginals (or, in other words, the magnetizations of the various spins). This because the “cavity system”, with respect to which marginalizations are performed, are slightly different, and because we need to disentangle the correlation functions. An approximation scheme is needed, and the Bethe approach is to consider decorrelation between marginal probability of spins around a cavity at site  $i$ :

$$p_{\partial i}^{(i)}(\sigma_{\partial i}) \stackrel{\text{Bethe}}{=} \prod_{j \in \partial i} p_j^{(i)}(\sigma_j) = \prod_{j \in \partial i} \frac{e^{\beta h_j^{(i)} \sigma_j}}{2 \cosh \beta h_j^{(i)}} \quad (3.8)$$

In such a way equation (3.7) could be solved as:

$$M_i^{(j)} \stackrel{\text{Bethe}}{=} \tanh \left\{ \beta h + \sum_{k \in \partial i \setminus j} \text{atanh} \left[ \tanh(\beta J) M_k^{(i)} \right] \right\}. \quad (3.9)$$

In particular for the homogeneous Ising Model, with degree  $2d = z$ , the mean-magnetization equations similar to (3.3) reads:

$$m = \tanh \left( \beta h + (z - 1) \text{atanh}(\tanh(\beta J) m) \right) \quad (3.10)$$

In particular for 1-dimensional lattice the calculation of critical temperature gives the expected result  $\beta_c = +\infty$ . Indeed, it could be proved that the Bethe Approximation is exact in dimension 1, as its interactions graph is a tree (actually a linear chain), and the decorrelation assumption is exact.

## 3.2 Cavity Method in general Replica Symmetric Models

Now we want to give a somewhat more systematic and general treatment of the previous derivation based on the framework of Cavity Theory.

As usual consider a model fully described by its Hamiltonian:

$$\mathcal{H}(\boldsymbol{\sigma}) = \sum_{a=1}^M E_a(\sigma_{i_1}, \dots, \sigma_{i_{k_a}}) + \sum_{i=1}^N W_i(\sigma_i) \quad (3.11)$$

where there are  $N$  variable site  $\sigma_i$  each in a proper one-particle space  $X_0$ , provided with a reference probability measure  $d\sigma$ . Functions  $W_i : X_0 \rightarrow \mathbb{R}$  represents  $N$  one-body interaction, while functions  $E_a : X_0^{k_a} \rightarrow \mathbb{R}$  represent a set of multi-particle interactions labelled by  $a \in \{1, \dots, M\}$ . As apparent the one-body interaction are extracted as requiring a particular treatment just for convenience reasons.

Quite naturally in such a picture a graphical structure emerges, that of a *factor graph*. This concept was introduced in Computer Science to study inference networks and could be described as follows. Given a factorization of a real function of real variables  $g : \mathbb{R}^N \rightarrow \mathbb{R}$ :

$$g(\mathbf{x}) = \prod_{j=1}^M f_j(x_{j_1}, \dots, x_{j_k}) \quad \text{with } \forall j, \quad f_j : \mathbb{R}^{k(j)} \rightarrow \mathbb{R}$$

we consider a bipartite graph  $G = (X, F, E)$  with  $N$  variable nodes, and  $M$  factor nodes, and a set of edges  $E \subset X \times F$ , such that node  $f_j$  is connected to node  $x_i$  if and only if the factor  $f_j$  has dependence from variable  $x_i$  with respect to (3.2).

Thus the factor graph associated to the Hamiltonian (3.11) is the corresponding factor graph of the joint probability measure. For our purposes this graph does not have factor of one-variable.

Consider now a minimal modification on the Hamiltonian (3.11) where it is switched off one link, say, the dependence of the variable  $\sigma_i$  on the interaction  $E_a$ . It should be noted that our statement is a bit more precise with respect to the “switching off” procedure in the Bethe approximation, there, in fact, the removed link did not belong to the factor graph, but just to the lattice (i.e., there the removing of an interaction involved modification to two links in the corresponding factor graph). Switching off procedure is done through the introduction of an auxiliary variable  $\sigma_{i_a}$  that substitutes the variable  $\sigma_i$  in the functional expression for  $E_a$ . Our interest in a minimal modification, leads to the choice of not associating any one-body term to the new auxiliary variable introduced, so the Hamiltonian reads:

$$\mathcal{H}_{a \leftrightarrow i}(\boldsymbol{\sigma} \cup \{\sigma_{i_a}\}) = \sum_i W_i(\sigma_i) + \sum_{b \neq a} E_b(\sigma_{\partial b}) + E_a(\sigma_{\partial a \setminus i}, \sigma_{i_a}) \quad (3.12)$$

where we used  $\partial a$  as the set of variable nodes adjacent to factor  $E_a$  in the original graph, and  $\partial a \setminus i$ , for the same set but element  $i$ .

Composition of this minimal modification procedure leads to systems in which all links from variable node  $i$  are removed, and those for which all links to the factor node  $a$  are suppressed. These systems are indicated as  $\mathcal{H}_{\setminus i}$  and  $\mathcal{H}_{\setminus a}$  respectively. In these systems, the contribution of site  $i$  or that from interaction  $a$  is fully decorrelated from the rest of the system, allowing thus a trivial factorization in the partition function.

Now, following the procedure for the Bethe approximation, our goal is to derive some relation between marginal probability distributions in the modified systems, and recovering a set of equations through some assumptions of decorrelation.

The marginal probability distribution could be reconstructed from a set of local observables over local observables  $\theta_i^\alpha(\boldsymbol{\sigma})$  where  $i$  runs with the variable sites, and  $\alpha$  parametrizes the set of observables needed for reconstructing the measure  $d\boldsymbol{p}(\boldsymbol{\sigma})$ , i.e., a basis in the space of normalized probability distribution over  $X_0$ . Clearly, if  $X_0$  has cardinality  $q$  (e.g. we can identify  $X_0 =$

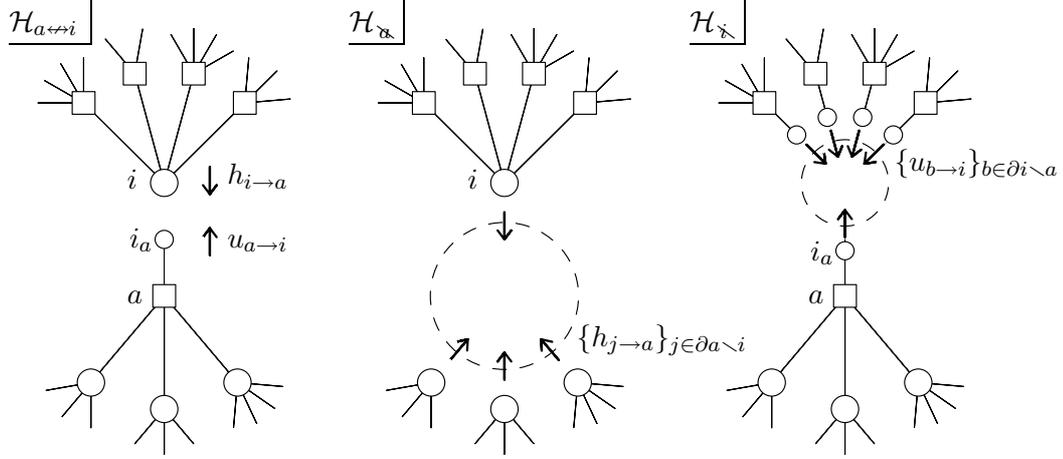


Figure 3.1: A portion of the factor graphs associated to the cavity Hamiltonians  $\mathcal{H}_{a \leftrightarrow i}$ ,  $\mathcal{H}_{\alpha}$ , and  $\mathcal{H}_{\hat{x}}$  respectively for the left, middle and right drawings.

$\{0, 1, \dots, q-1\}$ ), then  $q-1$  parameters will suffice, for example the vector  $(h_1, \dots, h_{q-1})$  will determine a normalized probability distribution over  $X_0$  through

$$p(x; h) = \begin{cases} \mathcal{N}^{-1} & x = 0 \\ \mathcal{N}^{-1} e^{-h_i} & x = i > 0 \end{cases} \quad \mathcal{N} = 1 + e^{-h_1} + \dots + e^{-h_{q-1}} \quad (3.13)$$

In simple magnetic systems, where the single-state space has just two values ( $X_0 = \{\pm 1\}$ ), a marginal distribution is parametrized by a single real number. Furthermore, if there is some underlying symmetry under inversion of all spins, it would be nice to preserve it “at sight” in the parametrization. Thus, in analogy with the case of an isolated magnetic spin subject to an external magnetic field  $h$ , we will parametrize in this case the probability distribution as

$$p(\sigma) = \frac{e^{\beta h \sigma}}{2 \cosh(\beta h)} \quad (3.14)$$

The terminology will thus be inspired by the one of magnetic systems, although we should keep in mind that more general parametrizations are possible, and the theory extends to these cases immediately.

So, Cavity Equations are usually expressed in term of such *generalized magnetic fields*:

**magnetic field  $h_i$** : the element  $h_i$  in the parameters space of probability distributions over  $X_0$  corresponding to the marginal probability distribution over site  $i$  in the original system  $p_{\{i\}}(\sigma)$  (in magnetic systems:  $p_{\{i\}}(\sigma) = p_{h_i}(\sigma)$ , with  $\tanh(\beta h_i) = \langle \theta_i(\sigma) \rangle$ ).

**cavity field  $h_{i \rightarrow a}$** : the element  $h_{i \rightarrow a}$  in the parameters space of probability distribution over  $X_0$  corresponding to the marginal probability distribution over site  $i$  in the modified system

where the link  $a \leftrightarrow i$  is switched off,  $p_{\{i\}}^{a \leftrightarrow i}(\sigma)$  (that is, in magnetic systems,  $p_{\{i\}}^{a \leftrightarrow i}(\sigma) = p_{h_{i \rightarrow a}}(\sigma)$ , with  $\tanh(\beta h_{i \rightarrow a}) = \langle \theta_i(\sigma) \rangle_{a \leftrightarrow i}$ , i.e., the expectation value of magnetization for site  $i$  for a system defined by Hamiltonian  $\mathcal{H}_{a \leftrightarrow i}$ ).

**cavity bias**  $u_{a \rightarrow i}$ : is the element in the parameters space for distribution over  $X_0$  that corresponds to the marginal probability distribution for the auxiliary site  $i_a$  in the system in which the inference channel  $a \leftrightarrow i$  is switched off,  $p_{\{i_a\}}^{a \leftrightarrow i}(\sigma)$  (that is, in magnetic systems,  $p_{\{i_a\}}^{a \leftrightarrow i}(\sigma) = p_{u_{a \rightarrow i}}(\sigma)$ , with  $\tanh(\beta u_{a \rightarrow i}) = \langle \theta_{i_a}(\sigma) \rangle_{a \leftrightarrow i}$  i.e., the expectation value of magnetization for the auxiliary site  $i_a$  for a system defined by Hamiltonian  $\mathcal{H}_{a \leftrightarrow i}$ ).

So, from an inspection of the marginal probability distribution in the various cavity systems, the following relations can be derived:

$$p_{\{i\}}^{a \leftrightarrow i}(\sigma) \propto p_{\partial i \setminus a}^{\times}(\sigma_{\partial i \setminus a}) e^{-\beta W_i(\sigma)} \quad (3.15)$$

$$p_{\{i_a\}}^{a \leftrightarrow i}(\sigma) \propto \int d\sigma p_{\partial a \setminus i}^{\boxtimes}(\sigma_{\partial a \setminus i}) e^{-\beta E_a(\sigma_{\partial a \setminus i}, \sigma)} \quad (3.16)$$

The proportionality factors in the relations above are not relevant in the RS treatment that we perform. They have a role in the ‘‘reweighting’’ factor, in 1RSB treatment, as they are in relation with the shift in free energy caused by the introduction/removal of a cavity in the system, and, in the case in which there are more pure phases in the system with different free energies, it would be important to weight them with the appropriate Gibbs factor.

For deriving the (RS) cavity equation is now necessary to introduce the decorrelation assumption:

$$p_{\partial i \setminus a}^{\times}(\sigma_{\partial i \setminus a}) \stackrel{\text{Cavity}}{=} \prod_{b \in \partial i \setminus a} p_{i_b}^{\times}(\sigma_{i_b}) \quad (3.17a)$$

$$p_{\partial a \setminus i}^{\boxtimes}(\sigma_{\partial a \setminus i}) \stackrel{\text{Cavity}}{=} \prod_{j \in \partial a \setminus i} p_j^{\boxtimes}(\sigma_j) \quad (3.17b)$$

alongside with the assumption that a larger cavity does not affect sensibly the marginal probability of variable sites far away from the cavity

$$p_{i_a}^{\times}(\sigma) \stackrel{\text{Cavity}}{=} p_{i_a}^{a \leftrightarrow i}(\sigma) \quad (3.18a)$$

$$p_i^{\boxtimes}(\sigma) \stackrel{\text{Cavity}}{=} p_i^{a \leftrightarrow i}(\sigma) \quad (3.18b)$$

These assumptions applied to equations (3.16) lead to the cavity equations:

$$\begin{cases} p(\sigma, h_{i \rightarrow a}) \propto e^{-\beta W_i(\sigma)} \prod_{b \in \partial i \setminus a} p(\sigma, u_{b \rightarrow i}) \\ p(\sigma, u_{a \rightarrow i}) \propto \int e^{-\beta E_a(\sigma_{\partial a \setminus i}, \sigma)} \prod_{j \in \partial a \setminus i} (p(\sigma_j, h_{j \rightarrow a}) d\sigma_j) \end{cases} \quad (3.19)$$

These equations allow in principle to determine the fields  $\{h_{i \rightarrow a}, u_{a \rightarrow i}\}_{(ia) \in E}$ , although one should face both the technical problem of solving a large system of non-linear equations (and proving that the solution is unique), and the “physical” problem of justifying the assumptions done alongside the derivation.

So, given the solution of (3.19), and within our assumptions, we can then reconstruct the marginal distribution for any site, in the original system. For example, for site  $i$ , taking any neighbouring factor node  $a$ , we would have that

$$p_{\{i\}}(\sigma) \propto p_{\{i\}}^{a \leftrightarrow i}(\sigma, h_{i \rightarrow a}) p_{\{i_a\}}^{a \leftrightarrow i}(\sigma, u_{a \rightarrow i}) \quad (3.20)$$

This would allow to determine recursively an exact sampling of the configurations, with the Gibbs measure at temperature  $\beta$ , and, as a corollary, to identify a ground state of the system, by performing the procedure in a limit  $\beta \rightarrow \infty$ .

It is worthwhile to spend here some more words on the physical nature of the assumptions above. The ones in equations (3.18) are relatively innocent, as well as all the paths which relevantly propagate inference from the cavity to the marginalized spin are long in comparison with the correlation length in the system. As the cavity is “nearby” to the spin in the original system, before creating the cavity, we identify the distribution of lengths for these paths with the one for the loops on the original factor graph. This assumption, on the fact that average loop lengths are sufficiently large, is crucial to all the method, and relatively well controlled on many natural families of random graphs (in particular, for *Erdős-Renyi* graphs with finite average degree, where typical loop lengths scale as  $\mathcal{O}(\ln N)$ ).

The assumption (3.17), on the fact that joint probabilities on more than one variable are almost factorized, relies on two points. One, again, is the assumption of “long loops”, which allows to state that the sites are on average far apart on the cavity system. The second one however is more subtle: in small words, it states that variables far apart do not interact relevantly, and thus their *connected* correlation functions are negligible. However, for statistical-mechanics systems which can undergo a phase transition, it is well known that this property holds *only within a pure phase*, and in particular it holds if we are in a region of thermodynamic parameters such that there is a single phase in the system (this fact is called *Cluster Property*). In order to see how this mechanism could fail, assume we have some local variable  $\sigma_i$ , in a homogeneous system, such that its average is a good order parameter for the system (i.e. that  $m = \langle \sigma \rangle$  assumes different values  $m_\alpha$  under different phases  $\alpha$ , in the region where the ergodicity is broken). Then we have that we can not hope  $p_{\{i,j\}}(\sigma_i, \sigma_j) \simeq p_{\{i\}}(\sigma_i) p_{\{j\}}(\sigma_j)$  if it is not true that at least  $\langle \sigma_i \sigma_j \rangle \simeq \langle \sigma_i \rangle \langle \sigma_j \rangle$ , but we have that each phase  $\alpha$  contributes to the convex combination with its factor  $\lambda_\alpha$  (so that, we recall,  $\lambda_\alpha \geq 0$  and  $\sum_{\alpha} \lambda_\alpha = 1$ ), in particular, in terms of the free energies  $F_\alpha$  inside a phase and  $F$  for the whole system, for the Gibbs measure we have  $\lambda_\alpha = e^{-\beta(F_\alpha - F)}$ . Then we

can see that

$$\langle \sigma_i \sigma_j \rangle = \sum_{\alpha} \lambda_{\alpha} \langle \sigma_i \sigma_j \rangle_{\alpha} = \sum_{\alpha} \lambda_{\alpha} \left( m_{\alpha}^2 + \langle \sigma_i \sigma_j \rangle_{\alpha}^{\text{conn.}} \right) \simeq \sum_{\alpha} \lambda_{\alpha} m_{\alpha}^2 \quad (3.21)$$

if  $|i - j| \gg \xi$ , where  $\xi$  is the correlation length in the system. Instead

$$\langle \sigma_i \rangle = \sum_{\alpha} \lambda_{\alpha} \langle \sigma_i \rangle_{\alpha} = \sum_{\alpha} \lambda_{\alpha} m_{\alpha} \quad (3.22)$$

so that

$$\langle \sigma_i \rangle \langle \sigma_j \rangle = \sum_{\alpha, \beta} \lambda_{\alpha} \lambda_{\beta} m_{\alpha} m_{\beta} \quad (3.23)$$

and in general the two quantities (3.21) and (3.23) will be in general different, unless we are in a pure phase, ( $\lambda_{\alpha^*} = 1$ , and  $\lambda_{\alpha'} = 0$  for  $\alpha' \neq \alpha^*$ , if any), so that both of them are just  $m_{\alpha^*}^2$ . An example where “things go wrong” is the Gibbs measure in a ferromagnetic Ising Model at temperatures showing spontaneous magnetization, where we have two phases with the same free energy and opposite  $m_{\alpha}$ , and the quantities (3.21) and (3.23) specialize to  $m^2$  and 0.

### 3.3 Cavity Method for the Assignment Problem

A “matrix” formulation of the Assignment Problem could be as follows: given  $\varepsilon$  a positive, real valued  $N \times N$  matrix defining the instance of the problem, we search for the  $N \times N$  matrix  $n_{ij}$ , valued in  $\{0, 1\}$ , which minimizes the cost function defined by

$$\mathcal{H}_{\varepsilon}(\{n_{ij}\}) = \sum_{ij} \varepsilon_{ij} n_{ij}. \quad (3.24)$$

Moreover, there are constraints on the set of feasible  $n_{ij}$ , in order to enforce the correspondence with a permutation, i.e.:

$$\{n_{ij}\} \in \mathcal{N}_N \quad \text{such that} \quad \forall j : \sum_i n_{ij} = 1 \quad \text{and} \quad \forall i : \sum_j n_{ij} = 1 \quad (3.25)$$

Thus a bijection exists from the space of permutations of  $N$  elements and the subset of  $GL_N(\{0, 1\})$  defined by (3.25):

$$F : \mathfrak{S}_N \rightarrow \mathcal{N}_N, \quad F(\pi) = \{n_{ij}\} \quad \text{with} \quad n_{ij} = \begin{cases} 1 & \text{if } \pi(i) = j \\ 0 & \text{if } \pi(i) \neq j \end{cases} \quad (3.26)$$

We can thus study the statistical properties of some random ensemble. We will choose a measure factorized over the entries,  $d\vec{\mu}(\{\varepsilon_{ij}\}) = \prod_{i,j} d\mu(\varepsilon_{ij})$ , furthermore we will assume that  $d\mu(\varepsilon)$  has support over some subset of  $\mathbb{R}^+$ , so that it is finite and continuous in  $\varepsilon = 0$ . Our concrete choice

in numerical analysis was just the flat measure over the interval  $[0, 1]$ , i.e.  $d\mu(\varepsilon) = \theta(\varepsilon)\theta(1-\varepsilon)d\varepsilon$ . A second interesting choice is  $d\mu(\varepsilon) = e^{-\varepsilon}d\varepsilon$ , which allows for a rigorous probabilistic analysis [12, 11].

Strong statements can be done for our problem, in order to justify this choice. A first trivial remark is the covariance of the problem under translation of the measure: if one uses  $d\mu'(\varepsilon) = d\mu(\varepsilon - a)$ , all the energies are shifted by a constant,  $Na$ , and all correlation functions between variables (e.g.  $n_{ij}$ ) remain unchanged. So, assuming that the minimum of the support is in 0, provided that the support is bounded from below, is not relevant.

A second qualitative remark is that a support bounded from below, and step-like in its neighbourhood, is indeed the most relevant case. A support with a “tail” on the left would create strong preferences towards certain choices: in turns, a fraction of the proper assignments  $n_{ij} = 1$  would be done with relatively small effort, w.r.t. our random case, while the remaining part of the problem will be just “typical”, but decimated. The case in which, in a neighbourhood of the left endpoint of the support (say, 0), the measure has a power law  $d\mu(\varepsilon) \sim \varepsilon^a$  has been studied in [13].

A last remark is the fact that, provided that the limit in 0 exists and is finite (together with its derivative), the  $k$  smallest values e.g. of a row (with  $\ln N \ll k \ll N$ ) will be distributed like the first  $k$  values of a *Poisson Point Process*, i.e., calling them  $(\xi_1, \dots, \xi_k)$ , we would have that  $\xi_1, \xi_2 - \xi_1, \dots, \xi_k - \xi_{k-1}$  would be i.i.d., and exponentially distributed,  $p(\xi) = a \exp(-a\xi)$ . As the constant  $a$  is the same for all rows and columns, and as the problem is on the reals, we understand that, if we prove consistently that the first  $k$  values are the only relevant ones for the statistical properties in a low-temperature regime, we also deduce that statistical properties of random ensembles which differ only in their limit  $\lim_{\varepsilon \rightarrow 0} d\mu(\varepsilon)$  are the same up to a trivial rescaling. This self-consistency proof can be done. For example, one finds that the probability that the  $k$ -th smallest value in a row participates to the optimal assignment is  $2^{-k}$ , in the limit of large  $N$ .

In physical terms, the problem of finding the minimal cost configuration, is related to the collapse of the allowed configuration in the limit for zero temperature onto the ground state, i.e., the state at minimal energy\*.

It is clear that, rigorously speaking, with a factorized measure over real numbers like the ones discussed above, there is zero probability (in “measure theory” sense) for having instances with a degeneracy, as the difference of cost between two configurations is a non-empty linear combination of the  $\varepsilon_{ij}$ ’s with coefficients in  $\{0, \pm 1\}$ . As we will see, and as is discussed in [2],

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\*In general many states of minimal energy could exist. In such a case we say that the ground state is *degenerate*. For example an Ising Model with inhomogeneous couplings  $J_{ij}$ , but no external field  $h$ , has at least two states of minimal energy, as configurations exchanged by the “global spin flip” transformation clearly have the same energy.

the absence of degeneracy plays some technical role in this problem, and even the Munkres' (or Knuth's) code, based on the Hungarian Algorithm, needs some extra procedure in order to deal with possible degeneracies. To be honest, the “analytic” justification above is a too cheap shortcut to the problem, and even the cheap justification of saying that there is no degeneracy up to adding some “infinitesimal” uncorrelated real-valued noise to the input instance, and then check back at the end that the solution is valid also on the original instance, in a weak argument, because, as intrinsic in the procedure of [2], the solution times diverge also if we have quasi-degeneracy, with an inverse power of the splitting between the two costs. Remarkably, this is not true for the Hungarian Algorithm, which is polynomial even in arithmetic encoding.

However we expect that a refined cavity algorithm, beyond the one depicted in [2] and in the direction of the “fork prescriptions” we use for slow instances, it should be possible in the degenerate case to obtain one solution in average-case times similar to the non-degenerate case, and all solutions in an instance with “moderate” degeneration  $g$ , in average times bigger just of a factor  $g$ , just following exhaustively the full forking procedure, and proving that the fork-to-solution ratio is bounded.

Here we just give a hint on how this potential problem of degeneracy is more “technical” than “structural”. Say that a non-trivial linear relation among the  $\varepsilon_{ij}$ 's, like the one discussed above for having degeneracy, is improbable with some small factor of order  $\delta$ , then one can argue that having degeneracy  $g$  is improbable with a factor of order  $\delta^{\lceil \log_2 g \rceil}$  or smaller. The reason for this is that the union of the symmetric differences for all the pairs of solutions is a subgraph (of the original complete bipartite graph) in which all vertices have degree different from 1 (as it is the union of cycles). If the cyclomatic number of this graph is  $L$ , then the probability of having such a graph is of order  $\delta^L$  (as the cyclomatic number is exactly the dimension of the space of pertinent linear relation among the parameters). But  $L$  is also the dimension of the space of functions, from the set of edges to  $GF(2)$ , satisfying some parity constraints at the vertices (i.e., the cardinality of the set of such functions is  $2^L$ ), while the set of effective solution is a subset of this, as the parity constraints are replaced by some consistent “ $\cdot = 1$ ” or “ $\cdot = 0$ ” constraints (1 for odd, and 0 for even). So that  $g \leq 2^L$ , equality being realized in the case in which the subgraph described above is a set of disjoint cycles (then the set of solutions is a hypercube w.r.t. the structure induced by symmetric difference).

Having discussed this technical point, we can now go back to the problem of specializing the general cavity framework of the previous sections to our problem of assignment.

Casting the cost function in the general form (3.11) for the statistical mechanics models, requires the introduction of interaction that force the space  $X = X_0^{N^2} = \{0, 1\}^{N^2}$  to satisfy the

constraints (3.25), so we introduce the following formal terms in the joint probability function:

$$\forall i \in \{1, \dots, N\} \quad e^{-\beta E_i^{(\text{row})}(n_{i1}, n_{i2}, \dots, n_{iN})} = \delta\left(\sum_j n_{ij}, 1\right) \quad (3.27)$$

$$\forall j \in \{1, \dots, N\} \quad e^{-\beta E_j^{(\text{col})}(n_{1j}, n_{2j}, \dots, n_{Nj})} = \delta\left(\sum_i n_{ij}, 1\right) \quad (3.28)$$

While the one-body terms just representing the cost of the assignment:

$$\forall (ij) \in \{1, \dots, N\}^2 \quad W_{(ij)}(n_{ij}) = \varepsilon_{ij} n_{ij} \quad (3.29)$$

The factor graph is thus composed of two kinds of interaction nodes, those for the constraints on the rows, and those for the columns, each joining  $N$  variable nodes. They are of the same nature, but globally identify a further bipartition of the set  $F$  of factor nodes in the graph. Consequently each of the  $N^2$  variable nodes is linked with two factor nodes, one ‘‘row’’ and one ‘‘column’’.

As variables live in a single-state space  $X_0 = \{0, 1\}$ , the marginal probability distributions are parametrized by a single real number:

$$p : X_0 \rightarrow \mathbb{R} \quad p(n) = \begin{cases} p_1 & \text{if } n = 1 \\ p_0 & \text{if } n = 0 \end{cases} \quad \text{with } p_0 + p_1 = 1 \quad (3.30)$$

For convenience our parametrization  $h$  is as follows:

$$p_1 = \frac{e^{-\beta h}}{1 + e^{-\beta h}}, \quad p_0 = \frac{1}{1 + e^{-\beta h}}, \quad \text{i.e., } p(n, h) = \frac{e^{-\beta h n}}{1 + e^{-\beta h}}, \quad (3.31)$$

where the probability which fixed a variable to 1 or 0 is the limit for the parameter  $h \rightarrow -\infty$  or  $h \rightarrow +\infty$  respectively. Considering the specialization of general notation for the AP:

$$\begin{cases} i \rightarrow (ij) \\ a \rightarrow i^{\text{row}} \text{ or } j^{\text{col}} \end{cases} \quad \begin{cases} \partial a \setminus i \rightarrow (ij') : j' \neq j \text{ or } (i'j) : i' \neq i \\ \partial i \setminus a \rightarrow j^{\text{col}} \text{ or } i^{\text{row}} \end{cases}$$

So the cavity equations (3.19) are  $4N^2$  equations binding an equal number of parameters of marginal probability distributions in  $X_0$ , i.e.,  $\{h_{(ij) \rightarrow i^{\text{row}}}, h_{(ij) \rightarrow j^{\text{col}}}, u_{i^{\text{row}} \rightarrow (ij)}, u_{j^{\text{col}} \rightarrow (ij)}\}$

$$\begin{cases} p(n, h_{(ij) \rightarrow i^{\text{row}}}) = f(n, u_{j^{\text{col}} \rightarrow (ij)}) \\ p(n, h_{(ij) \rightarrow j^{\text{col}}}) = f(n, u_{i^{\text{row}} \rightarrow (ij)}) \\ p(n, u_{j^{\text{col}} \rightarrow (ij)}) = g(n, \{h_{(i'j) \rightarrow j^{\text{col}}}\}_{(i'j) \in \partial j^{\text{col}} \setminus (ij)}) \\ p(n, u_{i^{\text{row}} \rightarrow (ij)}) = g(n, \{h_{(ij') \rightarrow i^{\text{row}}}\}_{(ij') \in \partial i^{\text{row}} \setminus (ij)}) \end{cases} \quad (3.32)$$

and using some algebra and the relation between the parameter and the probability values:

$$h = -\frac{1}{\beta} \log\left(\frac{p_1}{p_0}\right) \quad (3.33)$$

they could be written as:

$$\begin{cases} h_{(ij) \rightarrow i^{row}} = \varepsilon_{ij} + u_{j^{col} \rightarrow (ij)} \\ u_{j^{col} \rightarrow (ij)} = -\frac{1}{\beta} \log \frac{\sum_{n_{ij'}} \delta\left(1 + \sum n_{ij'}, 1\right) \exp\left(-\beta \sum h_{(ij') \rightarrow i^{row}} n_{ij'}\right)}{\sum_{n_{ij'}} \delta\left(\sum n_{ij'}, 1\right) \exp\left(-\beta \sum h_{(ij') \rightarrow i^{row}} n_{ij'}\right)} \end{cases} \quad (3.34)$$

and the corresponding ones with “row” and “col” interchanged, and matrix indices transposed.

In order to clean the notation for our problem, and solve the first trivial equation in (3.34), let's redefine the bias fields in a compact way:

$$\begin{cases} g_{i \rightarrow j} := u_{i^{row} \rightarrow (ij)} \\ h_{j \rightarrow i} := u_{j^{col} \rightarrow (ij)} \end{cases} \quad (3.35)$$

Then the cavity equation for the AP could be expressed in terms of  $2N^2$  equations for the bias fields only

$$\begin{cases} g_{i \rightarrow j} = \frac{1}{\beta} \log \sum_{j' \neq j} e^{-\beta(\varepsilon_{ij'} + h_{j' \rightarrow i})} \\ h_{j \rightarrow i} = \frac{1}{\beta} \log \sum_{i' \neq i} e^{-\beta(\varepsilon_{i'j} + g_{i' \rightarrow j})} \end{cases} \quad (3.36)$$

Taking the limit  $\beta \rightarrow \infty$ , they reduce to:

$$\begin{cases} g_{i \rightarrow j} = \max_{j' \neq j} (-\varepsilon_{ij'} - h_{j' \rightarrow i}) \\ h_{j \rightarrow i} = \max_{i' \neq i} (-\varepsilon_{i'j} - g_{i' \rightarrow j}) \end{cases} \quad (3.37)$$

## Chapter 4

# Analysis of the discrete map

In this chapter we concentrate on the discrete-time map for the bias fields derived from the Cavity Equation (3.37). In a first moment some details of the possible implementations are considered, and the interpretation as algorithm of *Belief Propagation* (BP) is described. Then an analytical and numerical investigation on the distribution of bias fields at zero temperature and at finite size is presented.

### 4.1 Parallel or Sequential update

Solving the Cavity Equations (3.37), even in RS framework and at zero temperature, is in principle a hard task. Indeed, the equations are not linear, except that in those neighbourhoods in which the argmax of the equations do not change (but there is in principle a huge number of those regions,  $\sim N^{4N}$ ), and some numerical idea should be adopted. A common tool in this case is to reinterpret the consistency equations as a dynamics, by introducing a fictitious time  $t$ , integer-valued, and write that the fields at time  $t + 1$  (the ones on the left side of the (3.37)) are some functional, complicated and non-linear but well known, of the ones at time  $t$ .

$$\{g_{i \rightarrow j}, h_{j \rightarrow i}\}^{(t+1)} = \Phi\left(\{g_{i \rightarrow j}, h_{j \rightarrow i}\}^{(t)}\right) \quad (4.1)$$

Then, iterating the map is computationally easy, and all the difficulty is concentrated on understanding how and why such a map could eventually reach a fixed point, and this should correspond, among the possibly-many fixed points, to the physically-relevant one.

Different implementations of the dynamics could lead to different average-case behaviour of convergence, and, as this issue is theoretically not well controlled, some heuristics and the sake of experience should be used. Common wisdom is that the so-called *sequential update*, in which at every time step a single field, picked at random, is updated according to its Cavity Equation, should give less stress to the pathological feedback effect due to short loops in the graph (which

make the true-life problem more distant from the realization on a tree, where the method would have been exact), and furthermore should avoid some collective modes which could arise in the opposite choice, of simultaneous update of all the fields (*parallel update*). For this reason, the sequential update is often the favourite one.

It pays, of course, the fact that now the method is intrinsically randomized, as in the definition of the dynamics we need to pick up indices in a set. Conversely, the sequential update can be made randomized, for example by choosing randomly the initial conditions, but it is also well-defined as a deterministic procedure (for example, starting from all zero fields).

As we will see, our problem is a remarkable exception: while the sequential update works just decently well, the parallel update works so well that it can be turned into an exact algorithm, an exceptional characteristic for an optimization problem (in comparison, a decision problem is structurally easier, it suffices to find one solution in a possibly large set, while optimization requires to identify that single optimal configuration!). Indeed, the reason for this striking property is related to the one which often leads to disregard the option of parallel updating: the sensibility to feedback cycles. In our case, we can certificate that, although the dynamics suffers from strong oscillations due to the spurious information propagated along the cycles, there exists one privileged cycle, which “talks louder” than the others, and in which the travelling information causes a virtuous effect of reinforcement on the solution.

Another choice for a dynamics, possible in principle but not much widespread, is the one of continuous-time dynamics. Instead of modifying an equation into a discretized dynamics like

$$\vec{x} = \Phi(\vec{x}) \tag{4.2}$$

into

$$\vec{x}(t+1) = \Phi(\vec{x}(t)) \tag{4.3}$$

one can take the variant

$$\vec{x}(t+dt) = \vec{x}(t) + dt(\Phi(\vec{x}(t)) - \vec{x}(t)) \quad \longrightarrow \quad \frac{d}{dt}\vec{x}(t) = \Phi(\vec{x}(t)) - \vec{x}(t) \tag{4.4}$$

There is an obvious reason for this: if the functional  $\Phi$  is complicated, integrating a differential equation is computationally heavy, and, although convergence and stability issues of continuous maps are often easier to address than the analogous for discrete times (as one can rely on continuity of the evolution, and on the fact that flow lines do not cross), these theoretical advantages tend to be negligible w.r.t. the numerical disadvantages.

Our case is an exception also under this aspect: the fact that the equations are locally linear, except that at those interfaces where some argmax changes, makes the integration of the continuous-time dynamics an easy task interval by interval. Again, this dynamics can be defined

in a deterministic way, so it is in a sense more similar to “parallel”, than to “sequential”, so it has some hope of leading, at least in principle, to an exact algorithm.

We believe that it is the case, although the work on this point is still in progress. As a hint of this fact, consider the following construction. At each time  $t$ , there is a certain set of argmax in the equations, which identifies a web of “who propagates messages to whom”. This web is a subgraph of the original graph, and, more precisely, it is an oriented subgraph, in which the in-degree of each vertex (who am I listening to) is 1 except that at an interface, and thus the out-degree is 1 on average. Thus, neglecting some exceptional points, this graph has no more than one cycle per component (we call these components “unicycles”. The time dynamics is solved by some easy spectral techniques, by introducing a proper Fourier basis, and it results that the lowest frequency is associated to the alternated-sign sum of the weights along the cycle. There is however a factor  $1/\ell$ , if  $\ell$  is the length of the cycle, due as always to the normalisation in the Fourier anti-transform. So, surprisingly, we recover the expression for the *drift*  $\Delta$  which is discussed in section 5.2.

Still, differently from the discrete-time algorithm discussed there, there is now a chance for making the algorithm polynomial even in algebraic encoding. Suppose that we have an exceptionally slow instance, because  $\Delta$  is very small: we need to perform many time iterations before the message from the cycle is sufficiently enforced. Nonetheless, for long sequences of these steps, the argmax in the equations are maybe constant, so the analytical integration of the continuous-time dynamics, extrapolated up to a point where some argmax changes, could speed up the procedure.

From the Cavity Equations (3.37) for bias fields can be easily derived a discrete time iterative map, hoping that for some domain it will eventually converge to a fixed point which determine a set of bias fields solving the Cavity Equations.

## 4.2 Belief Propagation interpretation

Belief Propagation (BP) Algorithm refers, in a narrow sense, to an iterative procedure of message passing between nodes in a Bayesian network, which allows to efficiently solve a certain class of inference problems [14, 15, 16]. In a wider sense, it refers to a class of algorithms (also called *Sum-Product*), developed in a number of different contexts, which have been recognized to have a common root, and the potentiality of being applied in a broader context of situations, only in recent times.

We will concentrate on the Sum-Product terminology\*, because it is the most useful for our

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\*As opposed to that of Bayesian inference networks, Markov Pairwise Fields, etc. see, for example [14], [15], [16].

purposes. The main problem is that of calculation of marginals of functions provided with a factorization. Given  $g(\mathbf{x})$ , a real valued function of  $N$  variables, suppose one can produce a factorization of it, in *local factors*  $\{f_j\}$ , depending on subsets  $X_j$  of the set  $X = (x_1, \dots, x_N)$  of variables, where  $j$  runs on some set  $J$ :

$$g(X) = \prod_{j \in J} f_j(X_j) \quad (4.5)$$

In a factorization naturally emerges, as said in section 3.2, a corresponding factor graph, in our case with  $N$  variable nodes and  $|J|$  factor nodes. Marginals  $g_i : X \supset \{x_i\} \rightarrow \mathbb{R}$  are defined in the same way as marginal probability distribution, except for the normalization requirement:

$$g_i(x_i) = \sum_{X \setminus \{x_i\}} g(X) \quad (4.6)$$

The key observation for the Sum-Product Algorithm is that in a cycle-free factor graph its structure provides an operational indication of how to perform marginal calculations, thanks, basically, to the distributive law of sum and product. This operative guide consists in transforming the factor graph in a tree rooted in  $x_i$ , so that a “parenthood” relationship is well defined for each node (i.e., pictorially like if the rooted tree is a genealogical tree). Let  $\mu_{x \rightarrow f}(x)$  a message from the variable node  $x$  to the factor node  $f$ , and  $\mu_{f \rightarrow x}(x)$  a message on the same edge in the factor graph but in reversed direction. Then the updating rules are:

$$\begin{cases} \mu_{x \rightarrow f}(x) = \prod_{h \in \partial x \setminus f} \mu_{h \rightarrow x}(x) \\ \mu_{f \rightarrow x}(x) = \sum_{X \setminus \{x\}} \left( f(X) \prod_{y \in \partial f \setminus x} \mu_{y \rightarrow f}(y) \right) \end{cases} \quad (4.7)$$

In order to compute marginal at variable site  $x_i$  is now required a message passing procedure along following this procedure:

1. Start from the leaves: each variable node sends an identity function to its parent, while each factor node sends itself.
2. Variable node sends products of messages arriving to it from its children.
3. Factor node  $f$  with a parent  $x$  forms the product of  $f$  with all messages coming from its children, and operate a summation over every variable but  $x$ , then pass it to its parent.
4. Marginal at  $x_i$  is calculated as product of all messages hitting  $x_i$  at any time.

The Sum-Product algorithm is based on the above procedure for computing all marginals in the factor graph, but lacking in this case a unique parenthood relationship, the parenthood is defined dynamically, so that any node first receives messages from all of its “children”, then pass a message to the remaining neighbour, its “parent”:

1. All leaf nodes send messages to their parent.
2. Every node waits for messages coming from all its neighbours but one, let's call this one its "parent", then it pass the computed message to the parent.
3. When the parent talks back it recompute the messages for each of its "children".
4. The procedure terminates when all the edges in the factor graph have broadcasted a message in each of the opposite directions.

Moreover the number of time steps in which all nodes become in condition of talking\* is twice the diameter of the tree, i.e., the length of the longest path between two nodes.

At the final stage, the marginals, or the *beliefs* in BP terminology, are then computed as sum of all messages received by a variable node:

$$\text{BEL}(x_i) = \sum_{f \in \partial x_i} \mu_{f \rightarrow x_i}(x_i) \quad (4.8)$$

A *Max-Product* algorithm refers to a very close technique in which sums at factor nodes are replaced by max operations. In this manner the purpose is not the calculation of marginals, but that of the maximally probable configuration. As it should be clear, maximization of marginals values does not imply any maximum probable *global* configuration. *Max-Sum* algorithm, in turn, is a variant that uses logarithms. Then, exploiting the monotonicity of logarithm and its formal properties, leads to replace products with sums which are computationally more efficient.

It should not be a surprise, then, recognizing that the Cavity Algorithm in its Replica-Symmetric formulation is essentially a Sum-Product algorithm, where cavity bias fields should be interpreted as messages running from factor nodes to variable nodes. Furthermore, the zero-temperature limit would correspond to the simplification of Max-Sum.

In particular, for our Assignment Problem, the updating rules in the Max-Sum algorithm are indeed the same as in the Cavity Equations we studied. Moreover, as in the factor graph the connectivity of variable nodes is equal to 2, their update rule is trivial, and it allows us to consider only bias fields in the procedure.

Of course, our problem seems ill-posed as BP, as the factor graph is not a tree-like structure, a situation that someone calls Loopy Belief Propagation (LBP). The theoretical status of LBP is far less clear than that of standard BP: as a matter of fact, messages could carry endlessly information through the cycles, giving rise to awkward beliefs convergence issues. For some models, in some ensembles, it may converge, while in other cases it may not, and it is not clear at this time if there exist and, in the case, which are, the conditions granting a good behaviour

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\*That is, a node should compute and pass messages to another if it just received all but one message from its neighbours, or it just received an "answer" from that neighbour to which it passed a message in a previous step.

under BP algorithm. The physical intuition on this point is that BP could hope of finding a good approximation of the marginals in a system, in the case in which the loops are sufficiently long on average, and in which there is a single pure phase in the system (i.e., there is no replica symmetry breaking), although these reasoning are still quite speculative, and could have exceptions.

### 4.3 The distribution of bias fields

In order to derive the expected distribution of bias fields during the iterations of the recursive map, consider the exact Cavity Equations for bias fields at zero temperature:

$$\begin{cases} g_{i \rightarrow j} = \max_{j' \neq j} (-\varepsilon_{ij'} - h_{j' \rightarrow i}) \\ h_{j \rightarrow i} = \max_{i' \neq i} (-\varepsilon_{i'j} - g_{i' \rightarrow j}) \end{cases} \quad (4.9)$$

In the thermodynamic limit, the expected distribution of fields is derived by solving the following distributional equation:

$$x \stackrel{d}{=} \max_i (-\xi_i - x_i) \quad (4.10)$$

where  $\{\xi_i\}$  is a Poisson Point Process (PPP) of rate  $\theta(\xi)$  and both  $x$  and the  $\{x_i\}$ 's are distributed i.i.d. with  $f(x)$ , a probability measure to be determined self-consistently.

The function  $f$  is found as follows. The random variables  $\{\xi_i + x_i\}$  are distributed as a PPP with rate given by the convolution product  $(\theta * f)(x)$ . Then, called  $F$  the primitive function of  $f$ , the probability that the value  $x$  is the maximum in a PPP with rate  $F(-x)$  is clearly proportional to the probability of the joint event that the value  $-x$  occurs and the probability of zero occurrences of values greater than  $-x$ :

$$\text{Prob}(x \text{ is maximum}) \propto F(-x)P_R(0) \quad \text{with} \quad \begin{cases} P_R(k) = e^{-R} \frac{R^k}{k!} \\ R = \int_x^\infty dt F(-t) \end{cases} \quad (4.11)$$

Some algebraic manipulation leads to:

$$f(x) = F(-x)e^{-\phi(-x)} \quad \text{with} \quad \begin{cases} F'(x) = f(x) \\ \phi'(x) = F(x) \end{cases} \quad (4.12)$$

This equation is ‘‘bilocal’’, i.e., besides depending on  $f$ ,  $F$  and  $\phi$ , thus being a differential equation, it depends both on  $x$  and  $-x$ . Some tricks facilitate the analysis: integrating both sides one gets  $F(x) = e^{-\phi(-x)}$ , then, taking the ratio of the two equations, one determines that  $f(x) = F(x)F(-x)$ , so one can state that  $f$  is symmetric, and  $F(-x)$  can be replaced by  $1 - F(x)$ . This makes the equation genuinely local, and the differential equation can be solved. One recognizes

in the solution a special function named *logistic distribution*, and its first and second primitive functions:

$$f(x) = \frac{1}{4 \cosh^2(x/2)} = \frac{e^x}{(1 + e^x)^2} \quad (4.13)$$

$$F(x) = \frac{e^x}{1 + e^x} \quad (4.14)$$

$$\phi(x) = \log(1 + e^x) \quad (4.15)$$

From the distributional equation (4.10) one can deduce more than the distribution of the fields. For example one can obtain the distribution  $p(\xi)$  for the entry  $\xi$  on which the maximum of  $-\xi_i - x_i$  is realized. This is of interest, because it corresponds to the distribution of instance entries  $\epsilon_{ij}$  chosen in the solution, rescaled by a factor  $N$ , and thus from this distribution we can extract the average value of the minimum energy,  $\langle E_{\min} \rangle$ .

The probability  $p(\xi)$  can be found by independence of Poisson Processes. Say we ask for the probability  $p(\bar{\xi}, \bar{x})$  that the maximum value is realized for a given pair  $(\bar{\xi}, \bar{x})$ . The remaining entries  $(\xi_i, x_i)$ , conditioned to the presence of the entry  $(\bar{\xi}, \bar{x})$ , are still an independent point process with rate  $\rho(\xi, x) = \theta(\xi)f(x)$ , thus the maximum of  $-\xi_i - x_i$  over these remaining entries is still distributed with  $f(x)$ . So  $p(\bar{\xi}, \bar{x}) = \text{prob}(-\bar{\xi} - \bar{x} > x)$ , with  $x$  and  $\bar{x}$  i.i.d. with measure  $f(x)$ . After integration we find

$$p(\xi) = \theta(\xi) \int d\bar{x} \int dx f(\bar{x}) f(x) \theta(-\bar{\xi} - \bar{x} - x) = \theta(\xi) \frac{e^{-\xi} - 1 + \xi}{4 \sinh^2(\xi/2)}. \quad (4.16)$$

The average value of the minimum energy corresponds to the first moment of this distribution (the factor  $1/N$  for the rescaling of the entries cancels out with the factor  $N$  of the sum):

$$\langle E_{\min} \rangle = \int d\xi \xi p(\xi) = \frac{\pi^2}{6}, \quad (4.17)$$

which is the celebrated Parisi conjecture, now proved by Nair *et al.* [12].

One could question how the abstract infinite-size limit of the Cavity Equation implied by the distributional equations is related to the fields one experiences when really performing the analysis. What happens is that the shape of the distribution  $f(x)$  is well verified numerically, up to a time-dependent translation factor, which is indeed responsible for the Cavity Equations to find the exact ground state. This translation factor is nonetheless on average “small” in  $N$ , so that non-surprisingly the distributional equation does not predict it.

We can consider more carefully the iterative map derived from the Cavity Equations:

$$\begin{cases} g_{i \rightarrow j}(t) = \max_{j' \neq j} (-\epsilon_{ij'} - h_{j' \rightarrow i}(t-1)) \\ h_{j \rightarrow i}(t) = \max_{i' \neq i} (-\epsilon_{i'j} - g_{i' \rightarrow j}(t)) \end{cases}$$

It is clear that, at every step, the matrix  $h_{j \rightarrow i}^t$  for each column  $j$  will have only two values, say  $\{h_j^{(\max)}(t), h_j^{(\text{sec})}(t)\}$  (and the first one is repeated  $N - 1$  times) defined as below:

$$\begin{cases} h_j^{(\max)}(t) = \max_i(-\varepsilon_{ij} - g_{i \rightarrow j}^t) \\ h_j^{(\text{sec})}(t) = \text{2nd max}_i(-\varepsilon_{ij} - g_{i \rightarrow j}^t) \end{cases}$$

A similar argument goes for the matrix  $g_{i \rightarrow j}^t$ . The first of these two equations may be reasonably assumed similar to the distributional equation of the analytical model in the thermodynamic limit, provided that:

1. The matrices  $g_{i \rightarrow j}$  share the same distribution of  $h_{j \rightarrow i}$  (here the point is an assumption of independence from the initial choices for  $h_{j \rightarrow i}$ , for the equations are clearly symmetric with respect to the two matrices).
2. At least during the first iterations the distribution of  $h_j^{(\max)}$  is predominant over  $h_j^{(\text{sec})}$  in the compound distribution, because of its weight of  $(N - 1)/N$  against  $1/N$ .

We will see in section 5.1 that, instead, for long times the second point fails, because the “sec” fields will “speak” half of the times. This is not surprising, as, when we almost detected a solution, it is reasonable that the entries which speak are the most reasonable ones, among the  $N$  of a row, most of which clearly of too high weight.

Assumed that these two points are valid for some transient times, and not required anymore after, when the distribution will remain quenched up to translation, it is reasonable to expect a logistic distribution for the  $\{h_j^{(\max)}\}$ 's. But in this case also the second equation takes a simple form, because it is just the distribution of:

$$y = \text{2nd max}_i(-\xi_i - x_i)$$

where  $\{\xi_i\}$  are random variables from a Poisson Point Process of rate  $\theta(\xi)$  and  $\{x_i\}$  random variables i.i.d. with the logistic distribution.

We can derive the actual form for a generic distribution  $p_k(y)$  solving

$$y = k^{\text{th}} \max_i(-\xi_i - x_i)$$

of which the logistic is a special case,  $f(x) = p_1(x)$ . We have only to adapt equation (4.11) for non-zero integer values in the Poissonian distribution, yielding:

$$p_k(y) = f(y) \frac{\log(1 + e^{-x})^{k-1}}{(k-1)!} \quad (4.18)$$

In particular the expected distribution for  $h_j^{(\text{sec})}$  is given by:

$$p_2(y) = \frac{\log(1 + e^{-x})}{(1 + e^{-x})(1 + e^x)} \quad (4.19)$$

A remark about this function should be made for its average value:

$$\langle y \rangle = \int_{\mathbb{R}} dx x p_2(x) = -\frac{\pi^2}{6} \quad (4.20)$$

Together with the fact that the average value in  $p_1$ , i.e., in  $f$ , is zero because the function is symmetric, this result is allusive of the known result for the average minimum energy. This is more than a coincidence: we will see that a certain combination of “max” and “sec” fields leads to a weighted covering of the graph, in the Egerváry sense of section 2.3, so exactly at fixed instance the minimum energy is equal to (minus) the sum  $\sum_i (h_i^{(\text{max})} + g_i^{(\text{sec})})$ , averaged over a certain interval of times. So, the result above on the first value of  $p_2$  is now read as an independent check.

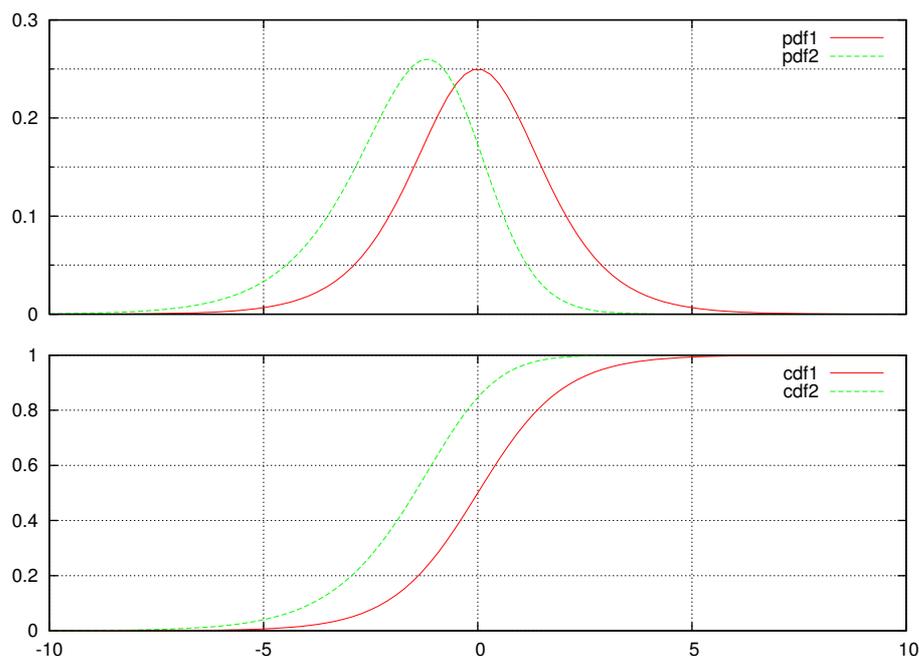


Figure 4.1: Expected distributions for  $h^{\text{max}}$  and  $h^{\text{sec}}$ .

We investigated numerically whether our expectations on the distribution of “max” and “sec” fields were right. A plot of these distributions and their cumulant is in figure 4.1, where the size of the instance is already such that the statistical noise on the data is not even recognizable with the eye.

These hypotheses agree well with the data from actual computations as shown in the figure (4.2) which reports the K-S test\* distance and significance level of the observed distributions with respect to the expected ones. In particular, one sees a rapid growth (on times of order 1) in the significance from the initial values (identically zeroes), followed by randomly fluctuating high values on some transient times, eventually taking a periodic behaviour, as a consequence of the fact that the set of fields itself becomes periodic, and we took out the overall translation.

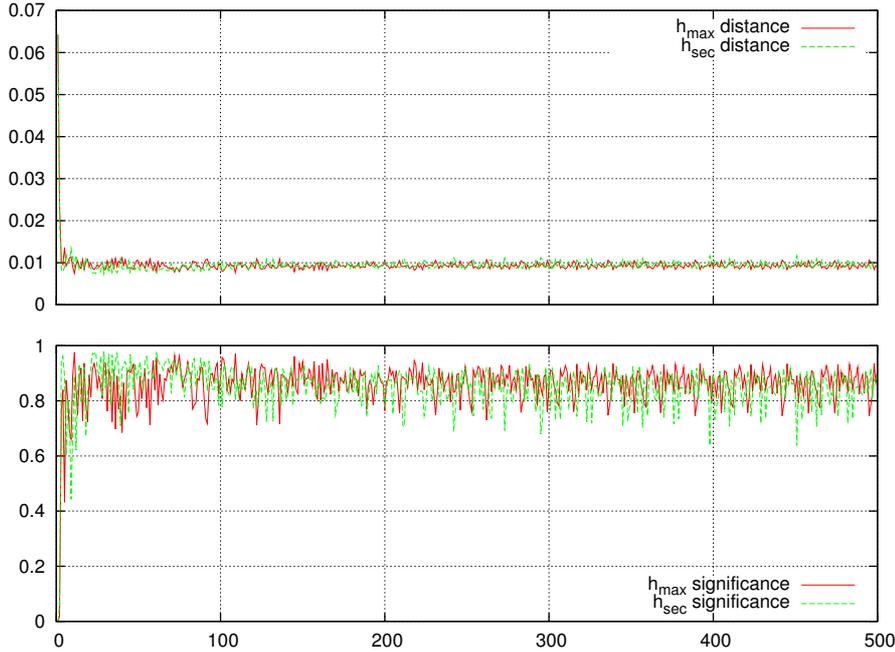


Figure 4.2: K-S distance and significance level between data and expected distributions for  $h^{(\max)}$  and  $h^{(\text{sec})}$  for an instance of size  $N = 4096$ .

A point is still a bit mysterious, on these parameters of translation: one combination of the two,  $\langle h^{(\max)} + h^{(\text{sec})} \rangle$ , has been already justified in terms of expected energy of the minimum, but the other combination, i.e., the extrapolation of  $\langle h^{(\max)} - h^{(\text{sec})} \rangle$ , which has asymptotically a linear behaviour, back to time  $t = 0$ , seems to be not constrained by any reasoning, and the prediction coming from the assumptions above seems to be wrong. Furthermore, this value seems to be not symmetric for  $h \leftrightarrow g$ , and not even self-averaging over the instances, for these reasons we interpreted it as a feature of the initial transient part in the cavity iterations, with small theoretical and practical significance.

Looking at the evolution of these average values and at their sum in figure (4.4), it is possible

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\*Kolmogorov-Smirnov test is a common tool to analyze the agreement between some data with an expected distribution. For a further treatment of K-S test see [18].

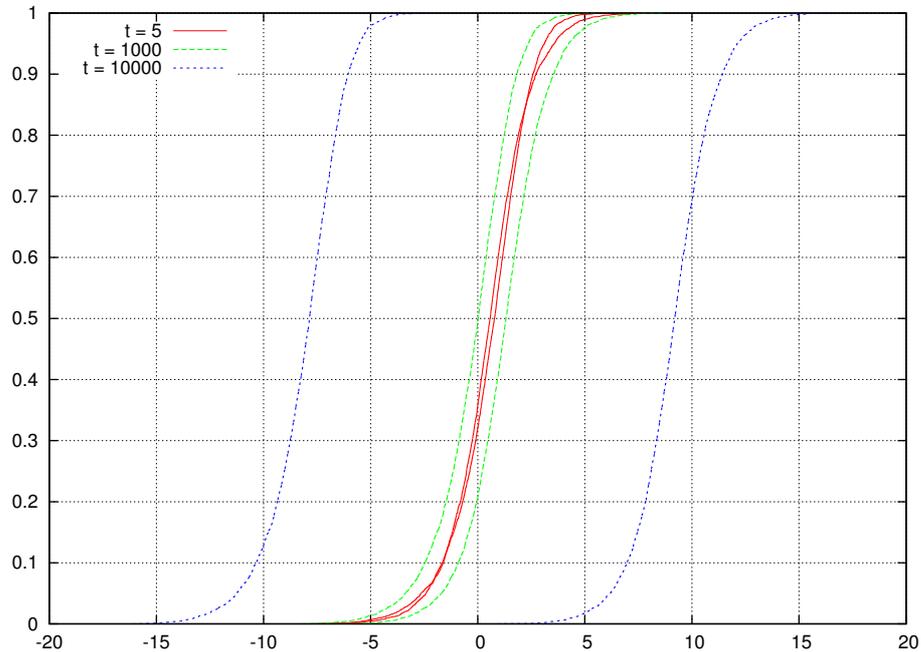


Figure 4.3: Cumulant distributions for  $h^{max}$  and  $h^{sec}$  for an instance of size  $N = 4096$  during the evolving of the recurrence map.

to see, after a transient stage a constant and periodic behaviour, suggesting a sort of freezing of the distributions of fields during some time in the transient phase. An inspection of this behaviour requires a better analysis of the mechanism through which the values of the Cavity Fields change during the recurrence map.

#### 4.4 Some remarks on the Replica Symmetry for the Assignment Problem

In all of this work, and mainly in using the Cavity Equations in our form, we assumed that the assumption of Replica Symmetry is correct for the Random Assignment Problem. There are many justifications of this fact, more or less heuristic, which can also be found in the literature, and we will discuss a few of them here. But, in particular, we will also show some “analytical proof”, in the framework of the full (modern) Cavity Theory, at the end of the section.

First of all, in the original replica calculation of Parisi and Mézard, the variational space of 1RSB solutions for the problem has a minimum at the RS point. These calculations are however both hard to follow, and partially hard to justify in all mathematical rigour.

Some numerical investigations have been performed some time later [19], and, although they

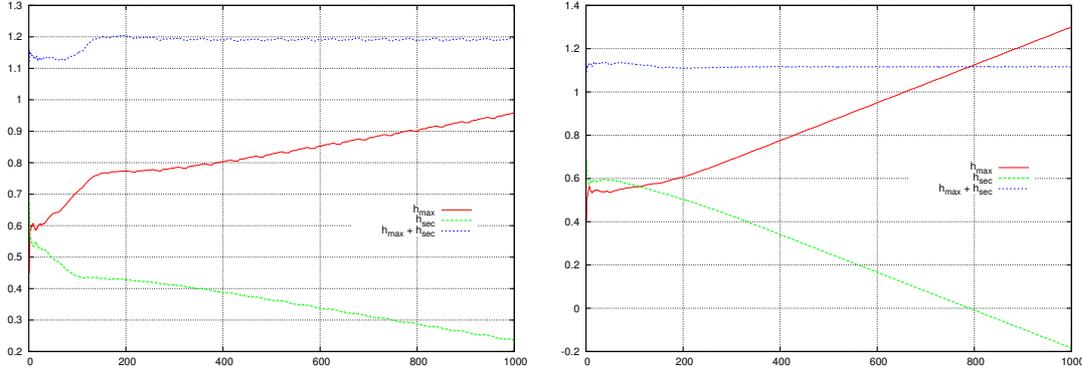


Figure 4.4: Average values for  $h^{max}$  and  $h^{sec}$  for two instances of size  $N = 4096$  during the evolving of the recurrence map. Where useful, a vertical offset between the curves has been adopted.

are not very extensive, they suggest however in a reasonable way that there is a single pure phase. We could easily reproduce for given instances, as a by-products of some of our codes, the distribution of the overlap on exactly the first  $\mathcal{N}$  configurations in the spectrum, and a few of these curves, at various sizes, are shown in figure 4.5

Indeed, also the algorithmic part of our work on the use of Cavity Equations as a solution algorithm, has, as a corollary, some implications on the fact that there should be a single pure phase – at least, with some “epsilon and delta’s”, in a certain finite-size analysis. Indeed, we proved that the (parallel update) Cavity Equations can identify the optimal matching starting from any initial conditions, thus proving that almost every measure on the phase space is dynamically attracted to the same fixed-point measure, which should thus describe the only basin of attraction with extensive size. The fact that this happens at “zero temperature” (i.e., in identifying the ground state) should imply that it happens *a fortiori* at finite temperature, because of basic thermodynamics disequalities (the disordered paramagnetic phase is always in a connected neighbourhood of the infinite-temperature point).

Furthermore, even the Hungarian Algorithm provides evidence for a single pure phase, although not so striking as with other argumentations. Indeed, consider the output of the algorithm, and the “transformed” instance, where entries are shifted by the Egerváry covering weights:

$$\varepsilon'_{ij} = \varepsilon_{ij} - \lambda_i - \mu_j \quad (4.21)$$

such that  $\varepsilon'_{i\pi(i)} = 0$  and  $\varepsilon'_{ij} \geq 0$  for all pairs (furthermore, in the ones we can construct through our covering function, of cavity fields averaged over a period,  $\varepsilon'_{ij} \geq \Delta$  for pairs  $(ij)$  not in the matching). Not only this certifies that  $\pi$  is optimal, but it also provides a strong intuition on

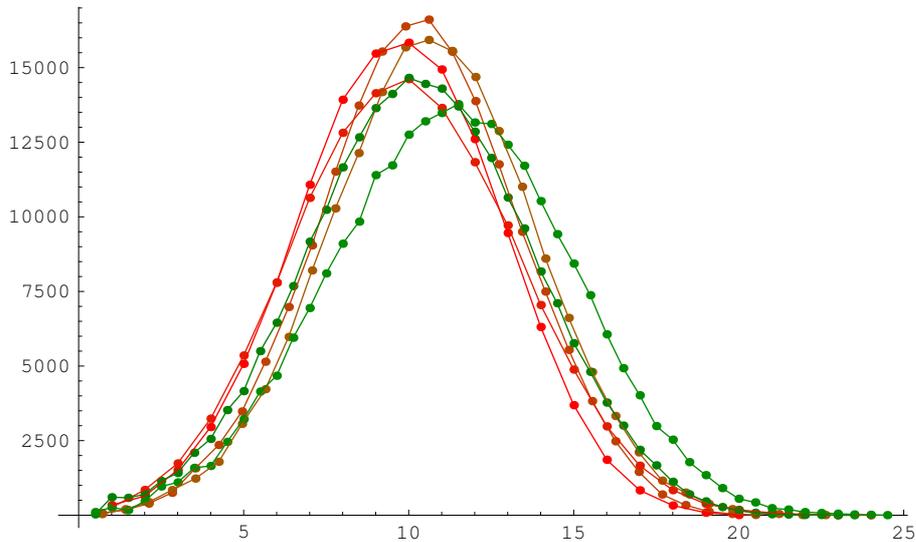


Figure 4.5: Distribution of the distance for all pairs of configurations, among the first 500 in the spectrum, for 6 random instances, 2 per size, at sizes  $N = 32, 64, 128$  (colours respectively red, orange and green). For sizes different from 32, a rescaling proportional to  $\sqrt{N/32}$  is understood. So, as the scaling exponent is  $1/2$ , i.e., smaller than 1, we recover the result of [19] on the fact that the distribution of the overlap tends to a delta in 1 for large sizes. The curves are well fitted by Gaussian curves, but the parameters seem to be a bit non-self-averaging, and the mean-to-variance ratio is not compatible with a binomial distribution.

the structure of the spectrum. The symmetric difference of any two matchings  $\pi'$  and  $\pi''$  is a set of disjoint self-avoiding cycles. Each of them contribute to the difference in cost of the two configurations, by the alternated-sign sum of the weights. If one of the matchings is the optimal one  $\pi$ , all these summands are positive. Indeed, all the intermediate configurations, in which some components are like in  $\pi$  and some like in  $\pi'$ , do exist, and if it were not the case that all the summands are positive, we would find a better matching among the intermediate ones. As a consequence, if a large fraction of relevant excited states at high distance from  $\pi$ , (or, more strongly, with one of the few low-energy states nearest to the ground state), it would hardly be possible that there are “valleys” far from the one containing  $\pi$ , because, given another local minimum, we would have a large number of configurations at intermediate distances, and with intermediate costs.

The idea of the existence of many components, if the distance is of order  $N$ , relies on an observation of the fact that closing alternating cycles on a good matching typically leads to cycles with length of order  $\sqrt{N}$  (cfr. for example the discussion and the data in section 6.2).

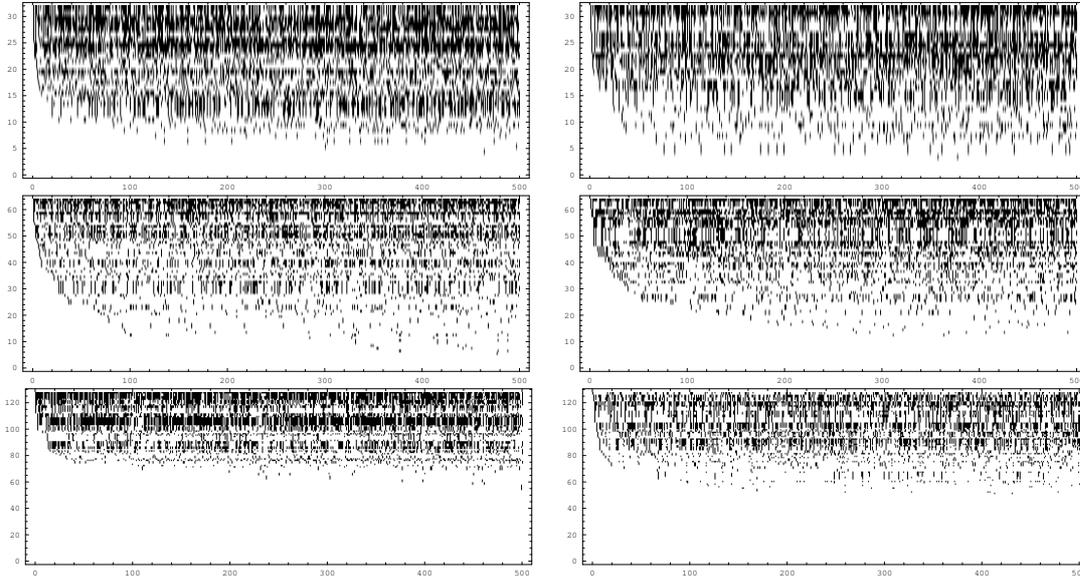


Figure 4.6: Diagrams for the overlap patterns with the ground state, for the instances in 4.5. Sizes are in increasing order from top to bottom. Remark the “strips” of indices with relative abundance of black entries.

So, this analysis does not exclude the possible appearance of “pseudo-1RSB” structures, with an anomalous finite-size scaling (with exponent  $1/2$  instead of  $1$ ) for the distances, so that the valleys correspond to alternating cycles on the optimal matching which are quite reasonable to switch.

More convincingly, we can show a representation of the full pattern of overlap with the ground state, obtained still by exact investigation of the spectrum: a black entry in row  $i$  and column  $j$  stands for the fact that entry  $\pi'(i)$  is different from  $\pi(i)$ , for  $\pi'$  being the  $j$ -th state in the spectrum, and the rows  $i$  have been ordered w.r.t. the structure of the diagram (topmost are rows which happen to be different from the optimal one before in the spectrum). For the same instances in figure 4.5, these graphics are reported in figure 4.6, while, for each row-index  $i$ , the fraction of the first 500 configurations in which it appears with a different matching w.r.t. the ground state makes histograms, which are reported in figure 4.7. Remark in this last figure how the curves fluctuate over many indices, corresponding to indices in the same cycle corresponding to some “translation” into a different “quasi-valley” with separation of order  $\sqrt{N}$  from the ground state.

Now we come to some less qualitative and more analytical treatment, although directly at infinite size, on the distributional equations. We know that the equation which determines the

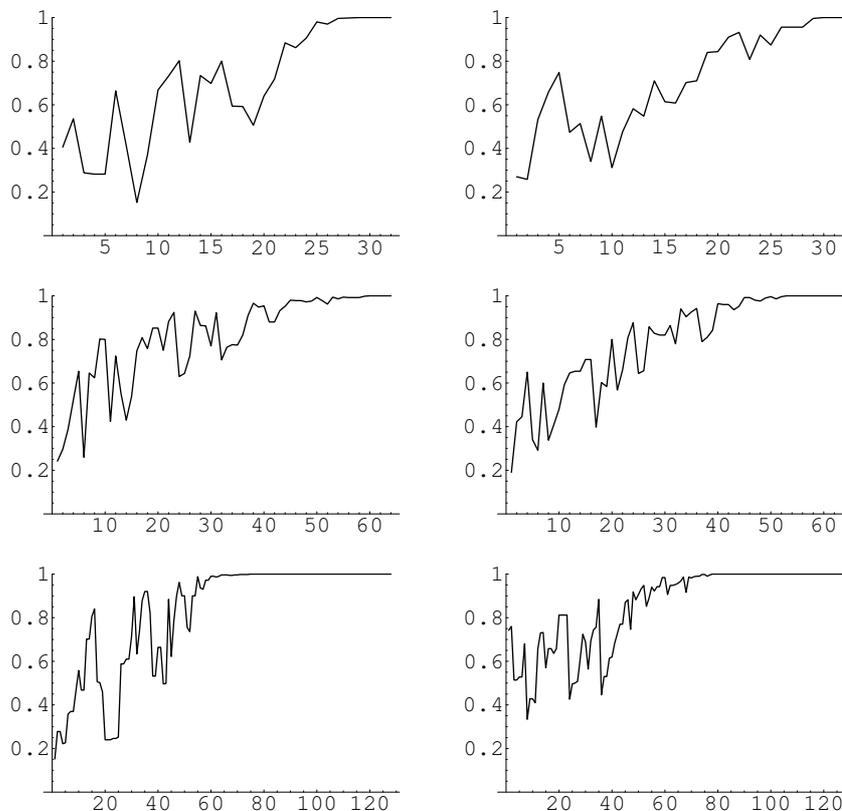


Figure 4.7: Histograms for the fraction of black entries in the diagrams of figure 4.6. They are quite non-self-averaging, in some allusive analogy with a Parisi function  $q(x)$ , and suggest some “quasi-valley” structure.

distribution of cavity fields is the following

$$x \stackrel{d}{=} \max_i(-\xi_i - x_i) \quad (4.22)$$

which come as a zero-temperature limit of the finite-temperature

$$x \stackrel{d}{=} \frac{1}{\beta} \ln \sum_i \exp(-\beta(\xi_i + x_i)) \quad (4.23)$$

A local-RS-stability criterion in the analysis of the equation for the cavity fields consists in studying how a local infinitesimal perturbation in the incoming fields (on the right side of the equation) propagates onto the outgoing field (on the left). The fact that the treatment is local allows us in turn to linearize the effect of the perturbation, so that we are reduced to study the spectral properties of some random linear operator: if all the eigenvalues are inside a disk of

radius 1, the effect is dumped, and a perturbation would not propagate, while if some eigenvalue is outside the disk, a perturbation with a non-zero component along the corresponding eigenvector would explode exponentially, and lead to an instability of the RS solution, typically interpreted as the possibility of many fixed points, in correspondence with the many pure phases of a 1RSB structure [20].

So, we call  $\epsilon_i$  the infinitesimal perturbations of the incoming fields  $x_i$ , and  $\epsilon$  the outgoing perturbation. We get

$$\epsilon = \sum_i \epsilon_i \frac{\partial x}{\partial \epsilon_i} = \sum_i \epsilon_i \frac{\exp(-\beta(\xi_i + x_i))}{\sum_j \exp(-\beta(\xi_j + x_j))} =: \sum_i \epsilon_i y_i \quad (4.24)$$

where we introduced a shortcut  $y$  for the derivatives. These quantities have the strong properties of being all positive at sight, and of summing up to 1. So, if we want to analyze whether the  $L_2$  norm of the fluctuations increases or decreases (we need to square them, because the average must be zero from the assumption of being at the fixed point of the distributional equation), we would get in the worst case

$$\max_{\{\epsilon_i\}} \frac{\epsilon^2}{\sum_i \epsilon_i^2} = \max_{\{\epsilon_i\}} \frac{\sum_{i,j} \epsilon_i (y_i y_j) \epsilon_j}{\sum_{i,j} \epsilon_i \delta_{ij} \epsilon_j} \quad (4.25)$$

i.e., the maximum eigenvalue of the rank-1 matrix  $M_{ij} = y_i y_j$  (which is obviously also the only one different from zero). Indeed we easily get for the characteristic polynomial

$$P(\lambda) = \lambda^{N-1} \left( \lambda - \sum_i y_i^2 \right) \quad (4.26)$$

but, as the  $y_i$  are all positive and sum up to 1, the sum of their squares is always smaller than 1, and equal in the case of a single value equal to one, and all the others vanishing. So the RS phase is always stable or at most marginally stable/unstable (still to be determined). Furthermore, it is easy to recover that the case of equality happens if one of the summands in (4.24) is dominant, which is always the case if the various  $(\xi_i + x_i)$  are different, and  $\beta \rightarrow \infty$ , i.e., in our zero-temperature random-real-ensemble case: we thus learn that RS is stable at finite temperature, and marginal at zero temperature. We can interpret this result of marginality as the distributional-equation signature of the “quasi-valley” structure qualitatively depicted above, where we lose the fact that the valley are separated by distances of order  $\sqrt{N}$ , instead of the appropriate extensive scaling, from the fact that the distributional equation has lost the subtler control on finite size.

The issue of marginality in the limit  $\beta \rightarrow \infty$  is a bit technical. Indeed, we have that the variation of  $\epsilon^2$  at the third order in the  $\epsilon_i$ 's is

$$2\beta \sum_{i,j,k} \epsilon_i \epsilon_j \epsilon_k (y_i y_j y_k - \delta_{ij} y_i y_k)$$

and, as evident from the study of the linear operator  $M_{ij}$  above, the most relevant direction, corresponding to the main eigenvector, is  $\epsilon_i = ky_i$ . In the limit of  $\beta \rightarrow \infty$  we can keep a vector  $y$  of the form  $(1 - a, a, 0, \dots, 0)$ , with  $a$  infinitesimal (and, say,  $b \equiv 1 - a$ ) and get for the variation (up to the positive factor  $2\beta$  overall) the expression

$$\begin{aligned} \sum_{i,j,k} \epsilon_i \epsilon_j \epsilon_k (y_i y_j y_k - \delta_{ij} y_i y_k) &= k^3 ((a^2 + b^2)^3 - (a^4 + b^4)(a^2 + b^2)) \\ &= k^3 (2a^2 b^2 (a^2 + b^2)) = k^3 \cdot 2a^2 (1 - a)^2 (1 - 2a) \quad (4.27) \end{aligned}$$

so, no surprises that the value of  $\epsilon$  increases/decreases if the sign of the main  $\epsilon_i$  is positive/negative, and, as the signs change at each passage, the overall effect is zero at this order (it had to, because odd terms can not survive), Nonetheless, this calculation was propedeutical to the one for the next even order, the fourth, for which we get, up to positive factors,

$$\sum_{i,j,k,h} \epsilon_i \epsilon_j \epsilon_k \epsilon_h (5y_i y_j y_k y_h - 8\delta_{ij} y_i y_k y_h + \delta_{ij} \delta_{kh} y_i y_k + 2\delta_{ij} \delta_{ik} y_i y_h)$$

Now factors of  $k$  come with an even power, and are not relevant. With calculations similar to the ones above, although more involved, one gets a polynomial in  $a$  of the form

$$-a(1 - a)(1 - 2a)^4(2 - 5a + 5a^2)$$

which is thus negative for infinitesimal values of  $a$ . From this we can conclude that also at  $T = 0$  the RS solution is marginally stable.



## Chapter 5

# Cavity equations as a “good” algorithm

In this chapter, the convergence proof for the discrete map is first outlined, and then rigorously proved. The proof uses some ideas of the Bayati, Shah and Sharma’s work [2], but enhances their conclusion with a better bound, and a really more precise set of statements about the stationary phase. This in turn, should be regarded as an useful addition, because convergence *per se* does not help in designing an algorithm which yearns for be an exact method. Instead a full description of the stationary dynamics could provide, and indeed does provide, expectations amenable of runtime check, in order to accomplish a halting condition.

### 5.1 Some remarks on the convergence mechanism

The numerical analysis of the bias fields emphasizes the following features:

1. the two sets of values  $\{h_j^{max}\}$  and  $\{h_j^{sec}\}$  are moving in opposite direction,
2. there is an instance-dependent speed, which, after a chaotic transient phase, converges to a clear value, eventually driving bias field values in a linear movement,
3. in the stationary phase, at large times, there is a periodic oscillation superimposed to the linear drift, with period instance-dependent, but shorter than the instance size.

Now we could write the 2-step map:

$$\begin{cases} g_{i \rightarrow j}^{(t)} = \max_{j' \neq j} \min_{i' \neq i} (-\varepsilon_{ij'} + \varepsilon_{i'j'} + g_{i' \rightarrow j'}^{(t-1)}) \\ h_{j \rightarrow i}^{(t)} = \max_{i' \neq i} \min_{j' \neq j} (-\varepsilon_{i'j} + \varepsilon_{i'j'} + h_{j' \rightarrow i'}^{(t-1)}) \end{cases} \quad (5.1)$$

and specializing it, in the long run assumption, i.e., when a separation of values is present, for proper indexes  $\bar{k}$ ,  $k$ ,  $\bar{l}$  and  $l$ :

$$\begin{cases} h_j^{max}(t) = -\varepsilon_{\bar{k}j} + \varepsilon_{\bar{k}l} + h_l^{max} \\ h_j^{sec}(t) = -\varepsilon_{kj} + \varepsilon_{k\bar{l}} + h_{\bar{l}}^{sec} \end{cases} \quad (5.2)$$

and similar equations for  $g^{max}$  and  $g^{sec}$ .

Let's introduce the indexes function related to the bias fields set  $\{h^{max}, h^{sec}, g^{max}, g^{sec}\}$ :

$$\begin{cases} l_i^{max}(t) := \arg \max_j (-\varepsilon_{ij} - h_{j \rightarrow i}^{(t-1)}) \\ l_i^{sec}(t) := 2nd \max_j (-\varepsilon_{ij} - h_{j \rightarrow i}^{(t-1)}) \end{cases} \quad \begin{cases} k_j^{max}(t) := \arg \max_i (-\varepsilon_{ij} - g_{i \rightarrow j}^{(t)}) \\ k_j^{sec}(t) := 2nd \max_i (-\varepsilon_{ij} - g_{i \rightarrow j}^{(t)}) \end{cases} \quad (5.3)$$

So it is reasonable to suppose that in the asymptotic behaviour are valid the following statements\*:

1.  $\{k^{max}, l^{max}\}$  becomes constant for large times, and they defines the optimal matching  $\pi$ , being one the inverse permutation of the other.
2. A subset of  $\{k^{sec}, l^{sec}\}$  also becomes constant, and their elements define, together with the previous permutation, a “competitive” matching  $\pi'$  on the complete bipartite graph, indicating the best alternatives to some of the elements chosen by  $\pi$ .
3. The difference between  $\pi$  and  $\pi'$  defines a cycle  $(i_1 j_1)(i_2 j_1)(i_2 j_2)(i_3 j_2) \cdots (i_1 j_p)$  of  $p$  ( $2 \leq p \leq N$ ) length, either  $\pi$ -alternating, and  $\pi'$ -alternating, with *minimal slope* which drives all  $\{h^{max}, g^{max}\}$  values to a positive and constant drift, and all  $\{h^{sec}, g^{sec}\}$  values to an identical drift, but with reversed slope.
4. the “stationary” behaviour is described by a small set of parameters coming from the best matching and an excited energy matching, with minimal drift defined as:

$$\Delta_{\pi'}^{\varepsilon} = \sum_{e \in \pi' \setminus \pi} \varepsilon_e - \sum_{e \in \pi \setminus \pi'} \varepsilon_e \quad (5.4)$$

So the stationary evolution of the map is reasonably assumed follow:

$$\forall t > t_0, \quad \begin{cases} h_j^{max}(t) = +\frac{\Delta_{\pi'}^{\varepsilon}}{p}t + C_j^{max}(t \bmod p) \\ h_j^{sec}(t) = -\frac{\Delta_{\pi'}^{\varepsilon}}{p}t + C_j^{sec}(t \bmod p) \end{cases} \quad (5.5)$$

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\*Indeed, they are also well-supported by numerical analysis

## 5.2 Proof of the main theorem

We recall the “parallel discrete-time iterated map” form of our cavity equations

$$\begin{cases} g_{i \rightarrow j}^{(t)} = \max_{j' \neq j}(-\varepsilon_{ij'} - h_{j' \rightarrow i}^{(t-1)}) \\ h_{j \rightarrow i}^{(t)} = \max_{i' \neq i}(-\varepsilon_{i'j} - g_{i' \rightarrow j}^{(t)}) \end{cases}$$

with the initial condition  $h_{j \rightarrow i} = 0$  at  $t = 0$  (or, more generally, some  $h_{j \rightarrow i}^{(0)}$  initial conditions). Say that the optimal matching (assumed here to be unique) is the one corresponding to the permutation  $\pi$ , so that, for  $\beta \rightarrow \infty$ , recalling that our  $g$ 's and  $h$ 's are “cavity biases” in the general language of section 3.2, the cavity fields identify the ground state if, for each  $(i, j)$ ,

$$\varepsilon_{ij} + g_{i \rightarrow j} + h_{j \rightarrow i} : \quad \begin{cases} < 0 & j = \pi(i) \\ > 0 & j \neq \pi(i) \end{cases} \quad (5.6)$$

What we will see is the stronger statement that, indeed, for any instance, the quantities above for the fields at time  $t$  will drift, linearly in time with some instance-dependent *drift* parameter  $\Delta$ , to  $\pm\infty$ , and with the proper signs in order to have that the quantities above diverge as  $\pm 2t\Delta$ .

Unfortunately, the parameter  $\Delta$  can be arbitrarily close to zero, and some refinements in the procedure are required in order to have effective convergence times.

We will be now more precise on what  $\Delta$  is. Given  $\pi$ , consider the set of all other permutations  $\pi'$ . Say that their “distance”  $\ell(\pi, \pi')$  is the number of indices  $i$  on which they differ (which is thus an integer in  $\{2, \dots, N\}$ ). It is indeed a good distance in the mathematical sense. Then, define the quantity  $E(\pi') = \text{cost}(\pi') - \text{cost}(\pi)$ , which is thus strictly positive because of our assumption of non-degeneracy of the ground state. Define  $(\Delta_1, \Delta_2, \dots, \Delta_{N-1})$  the ordered set of the  $\{E(\pi')/\ell(\pi, \pi')\}_{\pi' \in \mathcal{S}(N) \setminus \pi}$ . Then, our drift parameter is  $\Delta = \Delta_1 > 0$ , and only another combination,  $\Delta_{12} := \Delta_2 - \Delta_1$ , will play a role in the discussion. We will assume in the following that also  $\Delta_{12} > 0$ .

Remark that if the symmetric difference between  $\pi$  and  $\pi'$  has more than one component,  $E(\pi')$  takes a positive contribution from all the components. Put then in  $(E_1, \ell_1)$  the contribution to  $E$  and  $\ell$  coming from the first component, and in  $(E_2, \ell_2)$  the contribution from all other components. All of the four involved numbers are positive. This gives

$$\frac{E_1 + E_2}{\ell_1 + \ell_2} \geq \min\left(\frac{E_1}{\ell_1}, \frac{E_2}{\ell_2}\right) \quad (5.7)$$

which results from the fact that the two differences are both proportional to the same crossed factor  $(E_1\ell_2 - E_2\ell_1)$ , multiplied in the two cases by factors at sight of opposite sign. As a consequence, for the  $\pi'$  realizing the minimum  $\Delta$ , the symmetric difference with  $\pi$  must consist

of a single cycle. Similarly, for the  $\pi''$  realizing the second  $\Delta$ , it is either composed of a single cycle, or of two cycles, of which one is the one of  $\pi'$ .

Indeed, our aim is to prove that, by iterating the cavity equations above for a number of steps  $t$  larger than some constant, times some inverse powers of  $\Delta$  and  $\Delta_{12}$ , one reaches a situation in which the cavity fields  $h$  and  $g$  have some striking “quasi-periodicity” property, with period  $T$  equal to the distance  $\ell(\pi, \pi')$  for  $\pi'$  realizing  $\Delta_1$ . Averaging the final cavity fields over one period, one obtains some  $\{g_{i \rightarrow j}^{(\text{aver})}, h_{j \rightarrow i}^{(\text{aver})}\}$  which identify the optimal assignment  $\pi$  through the “sign” recipe described above, and provide a valid set of dual variables, in the sense described in section 2.3, which certifies the optimality of  $\pi$ . As a corollary, as the quasi-periodicity condition is easily tested on the run at every time step of the algorithmic procedure, this also provides a halting condition for the cavity algorithm, which was lacking in the original suggestion of [2].

The certificate is clear in its meaning: the combinations  $\{\varepsilon_{ij} + g_{i \rightarrow \pi(i)}^{(\text{aver})} + h_{j'(\hat{i}) \rightarrow i}^{(\text{aver})}\}$  (where  $j'(\hat{i})$  is some arbitrary index different from  $\pi(i)$ ) are exactly zero on the pairs  $(i, \pi(i))$ , and  $\geq 0$  on the other entries, and this proves at sight that  $\pi$  is optimal, as a restatement of the Egerváry’s theorem. It is interesting, also from the theoretical and speculative point of view, to remark the relation among the “physically inspired” cavity biases and the “computer science” dual variables, in particular at the light of the fact that rigorous understandings on the “heuristic” (and approximated on non-tree structure) cavity equations could allow to shed more light on their mechanisms, and maybe devise better strategies for applications even beyond the specific case of Assignment Problem.

All our statements above will be proved through a sequence of lemmas. The first one is contained in [2], and a few of the other ones either were in part implicit there but not stated, or are derived applying some variation of the two key ingredients:

- the correspondence with the tree-like unwrapped graph, and the fact that Belief Propagation is exact on that;
- the fact (obvious *a posteriori*, but still one should have had thought to that!), that paths on a finite graph, at the aim of the occupancy numbers on the edges, can be decomposed, e.g., through cycle-popping, into a set of self-avoiding cycles, and an open path of length smaller than the number of vertices in the graph.

So, given an integer  $t$ , an ordered pair  $(i, j)$ , and a “binary choice” among “row” and “col”, define the *unwrapped graph*  $\mathcal{T}(t; i, j, \text{“col”})$  (or the analogue for “row”) as the rooted tree, in which the root, at the top, is a copy of vertex “col  $j$ ”, it is connected only to a copy of vertex “row  $i$ ”, the latter is connected to other  $N - 1$  vertices, copies of “col  $j'$ ” for  $j' \neq j$ , each of them is connected to other  $N - 1$  vertices “row  $i'$ ”, for  $i' \neq i$ , and so on for  $2t$  levels ( $t$  with “row” vertices, and  $t$  with “col” ones). At the last level, we just have leaves. So we have a set of leaves (the last

level, plus the root), and a set of internal vertices, all of coordination  $N$ , and, w.r.t. the ordering induced by the rooting,  $N - 1$  of the neighbours are in a lower level, and one is in a higher level.

On this graph, it is understood a weight function on the edges, induced by the one on the original graph (if an edge in the unwrapped graph connects a copy of row  $i$  to a copy of col  $j$ , the weight is of course  $\varepsilon_{ij}$ ). For future use, we also define the function on the edges  $m_e \in \{0, 1\}$ , which is valued to 1 if the image of edge  $e$  on the original graph is occupied by the optimal matching. Then, we define a new matching problem on the unwrapped graph, stating that we search for the subset of edges such that:

- each internal vertex is covered exactly once;
- each leaf is covered either by one edge, or by no edges;
- the sum of the weights on covered edges is minimal in this set of feasible configurations.

A few observations can be done at this point. First, the cavity field  $\hat{g}_{i \rightarrow j}^{(t)}$  on the top edge-occupancy variable  $n_{ij}^{(t)}$  (coming from below, while from above the leaf do not send any message) coincides with the time- $t$  cavity field  $g_{i \rightarrow j}^{(t)}$  in the iteration of the equations for the original problem. Then, the cavity field for the unwrapped problem is *exact*, as we know that Belief Propagation is exact in this case.

The lemma states that

**Lemma 1** *If  $t \geq N \text{Const}/\Delta$ , where the constant is of small relevance and is discussed below, the sign of  $\hat{g}_{i \rightarrow j}^{(t)}$  is negative or positive respectively if  $\pi(i) = j$  or not.*

The proof works through a constructive absurd: if the thesis were false, one could build an alternating path on the unwrapped graph, connecting the root to one of the bottom leaves, such that, by studying the image of the path on the original graph, one would determine that inverting the occupancies on the path would improve the cost of the matching for the unwrapped problem, in disagreement with the fact that Belief Propagation is exact on the tree.

First we observe that, given any pair of allowed configurations  $n_1, n_2$  for the unwrapped problem, their symmetric difference is the union of some self-avoiding even-length cycles, and paths connecting two leaves, with edges occupied alternately in  $n_1$  and  $n_2$ . Call  $n_{(1)}$  and  $n_{(0)}$  the two optimal configurations, constrained to have respectively  $n_{ij}^{(t)} = 1$  or 0. Clearly, one of them is also the global optimum. Furthermore, for what we said above,  $n_{(1)}$  is the global optimum if and only if the sign of  $\hat{g}_{i \rightarrow j}^{(t)}$  is positive. The symmetric difference of  $n_{(1)}$  and  $n_{(0)}$ , that we denote with  $n_{(1)} \Delta n_{(0)}$ , must thus have a path connecting the root to some other leaf, and this path must be of length exactly  $2t$ . More precisely, as both configurations are optimal in their subensemble, the symmetric difference must be composed only of this path: no other paths between bottom

leaves, or cycles, are possible, because in one of the two cases there would be a net gain. A similar statement holds if we consider a third configuration, the one with  $n_{ij} = m_{ij}$ , built by unwrapping the optimal matching on the original problem\*. In this case, for both the symmetric differences of  $m$  with  $n_{(1)}$  and  $n_{(0)}$ , there could be an arbitrary number of disjoint paths, but no internal cycles. In  $n_{(1)} \Delta n_{(0)}$ , and one among the two  $n_{(1)} \Delta m$  and  $n_{(0)} \Delta m$ , there must be a path connecting the root to a leaf in the bottom, while the portions of the two paths which is not in common makes a path “bottom-to-bottom” in the other difference. (We neglect here the possibility that the optimum configuration is degenerate on the unwrapped problem. In this case one should modified the statement into “one can choose an optimal  $n_{(1)}$  and an optimal  $n_{(0)}$  such that...”.)

Another relevant point is the fact that this bottom-to-bottom path is bounded in length, by  $2N$ , because, if projected onto the original problem in such a way that it is not self-avoiding, it would lead to a gain move in the pertinent  $n_{(\cdot)}$ , without touching the occupancy at the root, thus contradicting the optimality hypothesis. So the part of the path in this “ $\lambda$ -shaped” diagram which goes from the crossing to the top is long at least  $2t - N$ .

The difference in cost between the two configurations is given by the alternated-sign sum of the weights  $\varepsilon_{ij}$  along the path. Here there is the crucial point: in the absurd hypothesis that the sign of  $\hat{g}$  is not in accord with the original-problem occupancy  $m_{ij}$ , the signs on the portion of the path of length larger than  $2t - N$  are alternating in such a way that on any closed cycle the loss is in the direction of contradicting the assumption of global optimality. On each closed cycle, the loss per level is at least  $\Delta$  (because of the definition of the quantities  $\Delta_i$ : remark how the division by  $\ell(\pi, \pi')$  was pertinent). On the other side, there is no contradiction still as long as the other summands could recover this loss. But, by a cycle-popping argument on the path, we see that both the contribution coming from the bottom part of the  $\lambda$ , and the one coming from what remains of the top part after the cycle-popping, are bounded by the difference in energy in the alternated-sign-sum along an open self-avoiding path on the original graph, and this quantity can be evaluated easily at given instance, then maximized over pairs  $(ij)$ , or otherwise bounded easily *a priori* by a factor proportional to  $N$  in the case of a bounded measure on the  $\varepsilon_{ij}$ . So, the loss can not be compensated for  $t$  sufficiently large w.r.t. this factor, proportional to  $N/\Delta$ . This concludes the proof of the lemma.  $\square$

However one should remark that the value of  $\Delta$  is both arbitrarily close to zero, and impossible to deduce from the instance, unless with some procedure which is essentially equivalent to solve the problem otherwise (e.g., by applying multiple times<sup>†</sup> in a smart way the Hungarian

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\*Remark that, as for internal vertices we have the same constraints as in the original problem, and on the leaves we have relaxed the constraint, this configuration  $m$  is in the set of feasible ones.

<sup>†</sup>Not being  $\Delta$  determined by the first excited state of the spectrum, it is not sufficient calculate it, but as much excited states as it needs for the last calculated excited energy divided by  $N$  is greater than the candidate

Algorithm), so we both do not have a bound on the running time, and not even a certified fixed-instance threshold time such that, stopping the algorithm after that time, we can safely conclude that the reconstructed matching is optimal.

For this reason we go further with our analysis of the mechanisms of the problem. We can call  $t^*$  a time sufficient at the purposes of lemma 1. As the cavity equations at zero temperature are of our special form  $\max_i(\dots)$ , it makes sense to consider the argmax at each node. Again for simplicity neglect the possibility that at some nodes there could be degeneracy (it could be nice to know that this never happens in measure for the case of random real-valued instances). Still, consider the messages propagating upwards, to the root of the tree. So we can say that, of the  $N - 1$  downward neighbouring edges, one of them is the “speaking edge”, if it is the one with label corresponding to the argmax of the Belief Propagation equations at that node and at the fixed point.

A simple fact is the following

**Lemma 2** *For each  $t \geq t^*$ , for all the first  $t - t^*$  levels of the tree (the nearest ones to the root), all the edges  $e$  with  $m_e = 1$  are speaking edges.*

This is implicit from the structure we constructed through the first lemma, plus the observation that, through the thesis of the lemma 1, the edges in the matching of the original problem send a message with positive sign, while all the other  $N - 2$  incident edges send a negative message.  $\square$

Still, this determines only “half” of the speaking edges: alternately along the path, the edge speaking to one such that  $m_e = 1$  is not still fixed.

Another useful remark, implicit in the consequences of the lemma, is the fact that, within the notations of section 4.3 where the fields  $g_i^{(\max)}(t)$  and  $g_i^{(\text{sec})}(t)$  are introduced (and analogously for  $h$ 's), we see that in the upper  $t - t^*$  levels of the tree, i.e., after  $t^*$  iteration steps on the original system, we are in a regime such that the “max” messages speak to “sec” ones and vice-versa.

We have now all the background necessary to prove the following

**Lemma 3** *For  $t > t^{**} = (\text{Const}_1 t^* + \text{Const}_2 N)/\Delta_{12}$ , where the irrelevant constants are described below, and for  $T$  being the length of the cycle realizing the drift  $\Delta$ , the set of cavity fields  $\{\hat{g}_{i \rightarrow j}^{(t)}, \hat{h}_{j \rightarrow i}^{(t)}\}$  have the quasi-periodicity property*

$$\hat{g}_{i \rightarrow \pi(i)}^{(t+T)} = \hat{g}_{i \rightarrow \pi(i)}^{(t)} - T \Delta; \quad \hat{g}_{i \rightarrow j}^{(t+T)} = \hat{g}_{i \rightarrow j}^{(t)} + T \Delta \quad \text{for } j \neq \pi(i); \quad (5.8)$$

$$\hat{h}_{j \rightarrow \pi^{-1}(j)}^{(t+T)} = \hat{h}_{j \rightarrow \pi^{-1}(j)}^{(t)} - T \Delta; \quad \hat{h}_{j \rightarrow i}^{(t+T)} = \hat{h}_{j \rightarrow i}^{(t)} + T \Delta \quad \text{for } i \neq \pi^{-1}(j). \quad (5.9)$$

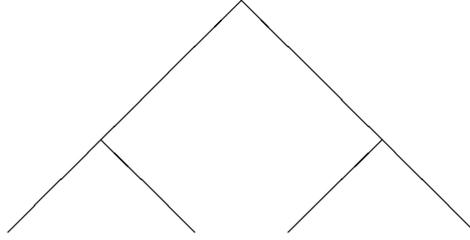
The proof could be conceptually divided into two steps. One is just technical, and analogous to the technique devised in lemma 1: it requires to prove that an alternating path from the new root 

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 drift to that moment.

to a level down to  $t^*$  from the bottom must go through the optimal cycle with drift  $\Delta$  for almost the whole fraction of its length, otherwise the loss for not doing so (but following, for example, the second-optimal cycle with drift  $\Delta + \Delta_{12}$ ) could not be compensated by the boundary effects of the self-avoiding open path resulting from the cycle popping.

The first step, however, should come before. Why should we care for some “global optimality” condition, like the fact that the result of flipping a whole path has definite sign, while the statement we want to prove concerns a cavity field, determined through a “local” procedure of who’s speaking to whom? This is the combined result of the small lemma 2 above, and of the fact that, because of the “max” nature of the 2-step cavity equations. Consider indeed a diagram like



where the segments stand for portions of alternating paths on the unwrapped graph, and the heights of the nodes where paths meet have the same parity (even). One can devise a global quantity on the paths from the root to some fixed level, obtained as a certain local combination of the costs on the crossed edges, in such a way that minimizing this quantity selects the path of speaking edges from the given layer to the root. Indeed, assume inductively that this is true up to a height  $2h$ , then we want to prove it up to level  $2h + 2$ . We can have a look back at the cavity equation, and nest them in two steps:

$$g_{i \rightarrow j}(t + 1) = \max_{j' \neq j} (-\varepsilon_{ij'} - h_{j' \rightarrow i}(t)) = \max_{j' \neq j} \left( -\varepsilon_{ij'} - \max_{i' \neq i} (-\varepsilon_{i'j'} - g_{i' \rightarrow j'}(t)) \right) \quad (5.10)$$

As we have a minus sign in between the two max operators, we can not reduce it to a simple maximization (which would have been an unrealistic trivialization of the procedure), and our idea of devising a global quantity to maximize, at least in this approach of looking at quantities which are natural in cavity framework, seems unfeasible. Nonetheless, as we said above, we are certificated in a regime such that “max” speak to “sec”, which speak to “max” and so on, and also, one every two indices is known rigorously to be the one suggested by the optimal matching  $\pi$ , so that we can specialize the equation above to this regime

$$g_i^{(\max)}(t + 1) = \max_{j' \neq j} (-\varepsilon_{ij'} - h_{j'}^{(\text{sec})}(t)) = \max_{j' \neq j} \left( -\varepsilon_{ij'} - 2\text{nd} \max_{i'} (-\varepsilon_{i'j'} - g_{i'}^{(\max)}(t)) \right) \quad (5.11)$$

(because the argmax over  $i'$  is realized on  $i$ ), so

$$g_i^{(\max)}(t + 1) = \max_{j' \neq j} \left( -\varepsilon_{ij'} + \varepsilon_{\pi^{-1}(j')j'} + g_{\pi^{-1}(j')}^{(\max)}(t) \right). \quad (5.12)$$

This expression proves our statement, on the fact that, at the aim of determining the value of the cavity field on the root at a certain time  $t$ , given the input cavity fields at level  $t^*$  from the bottom, it suffices to determine the (maximum value of the) alternated-sign sum of the weights on the path, starting from a leaf at this level and reaching the root. This is true simultaneously for all pairs  $(ij)$ . Furthermore, as the value of the field comes from the sum of local quantities on the graph, optimized in some way, it must be that for large times it reaches a linear regime (i.e., the one for which, for most of the time, it applies the optimal strategy). Finally, for every connected component (and, in our case in which all weights  $\varepsilon_{ij}$  are finite, definitely for all pairs), the slope of the linear regime must be the same for all the pairs.

A candidate for this slope is of course our drift parameter  $\Delta$ . We can easily construct, for example, a whatever path which reaches the drift cycle in some finite number of steps, then walks on it for all the time steps down to  $t^*$ . Then, as  $\Delta$  is the minimum drift, no other values are possible without violating the optimality condition. A “second better” condition is that almost all the paths follow, as much as possible, the optimal cycle, while one or more of them, for some time interval, follow the second-optimal cycle.

Consider now two cases:

- For some time interval  $\{t, t + 1, \dots, t + T\}$  all the paths have followed the optimal cycle. In this case, we would enter the quasi-periodic regime described above, as results evident from the cavity equations, specialized to the fact that “max” speak to “sec” and vice-versa.
- For all time intervals of the for above, at least one path has done at least one step out of the optimal cycle (say, in the sub-optimal one). Then, on average, the drift would be  $\Delta + \Delta_{12}/(T \cdot 2N) > \Delta + \Delta_{12}/(2N^2) > \Delta$  (remark, *strictly* larger), this violating our condition on the fact that the drift must be optimal.

This proves also the present lemma. A technical final point consists in estimating a time  $t^{**}$ , depending from  $\Delta_{12}$ ,  $N$  and the values of the cavity fields at level  $t^*$  (which are easily and generously bounded by a factor proportional to  $t^*$ ), and this leads to our estimate in the statement of the lemma.  $\square$

Now everything is essentially done: as we are forced to enter a quasi-periodic regime, and as such a fact is easily detected in an algorithmic implementation (for example, through a hash function of the kind

$$f_{\lambda}(g, h; t) = \sum_i (\lambda_i g_i^{(\max)}(t + 1) + \lambda'_i h_i^{(\text{sec})}(t)) \quad (5.13)$$

where the  $\lambda$ 'a are real numbers such that  $\sum_i \lambda_i = \sum_i \lambda'_i$  but have no other linear relation with rational coefficients), and as we know in this case that the asymptotic behaviour easily extrapolated from the argmax in the cavity equations will definitely lead, when  $t = t^*$ , to

identify the same optimal matching suggested by the present set of argmax indices, we have now a criterion for safely halt the procedure, and output the result.

Nonetheless, this idea of extrapolating up to  $t^*$  (which, in principle, could be larger than the time at which quasi-periodicity is detected) is a bit disturbing in its lack of elegance. We want to prove in a final lemma that, already through the fields in our interval of quasi-periodicity  $\{t, t+1, \dots, t+T\}$ , the optimal matching has been identified by the cavity equations because of some structural reason. Indeed we have

**Lemma 4** *In quasi-periodic regime, the quantities  $\{g_{i \rightarrow j}^{(\text{aver})}(t), h_{j \rightarrow i}^{(\text{aver})}(t)\}$  defined as*

$$g_{i \rightarrow j}^{(\text{aver})}(t) = \sum_{t'=t}^{t+T-1} g_{i \rightarrow j}(t'); \quad h_{j \rightarrow i}^{(\text{aver})}(t) = \sum_{t'=t}^{t+T-1} h_{j \rightarrow i}(t'); \quad (5.14)$$

*are a good set of dual variables, in the sense of section 2.3, and thus provide a certificate of optimality of the permutation  $\pi$  that they identify.*

Call  $\varepsilon'_{ij}$  the weights shifted by the dual variables, i.e.,  $\varepsilon_{ij} + g_{i \rightarrow j}^{(\text{aver})}(t) + h_{j \rightarrow i}^{(\text{aver})}(t)$ . We have to prove two statements, first that  $\varepsilon'_{i\pi(i)}$  is exactly zero for each  $i$ , then that  $\varepsilon'_{ij} \geq 0$  for each pair of indices. For the first case we have

$$\begin{aligned} \varepsilon'_{i\pi(i)} &= \varepsilon_{i\pi(i)} + \frac{1}{T} \sum_{t'=t}^{t+T-1} (g_i^{(\text{sec})}(t) + h_{\pi(i)}^{(\text{max})}(t)) \\ &= \varepsilon_{i\pi(i)} + \frac{1}{T} \sum_{t'=t}^{t+T-1} (g_i^{(\text{sec})}(t) + (-g_i^{(\text{sec})}(t) - \varepsilon_{i\pi(i)})) = 0 \end{aligned} \quad (5.15)$$

while for the second case, with  $j \neq \pi(i)$ , we have

$$\begin{aligned} \varepsilon'_{ij} &= \varepsilon_{ij} + \frac{1}{T} \left( h_j^{(\text{max})}(t+T-1) + g_i^{(\text{sec})}(t) + \sum_{t'=t+1}^{t+T-1} (h_j^{(\text{max})}(t-1) g_i^{(\text{sec})}(t)) \right) \\ &= \Delta + \frac{1}{T} \sum_{t'=t}^{t+T-1} (g_i^{(\text{sec})}(t) + (\varepsilon_{ij} + h_j^{(\text{max})}(t-1))) \end{aligned} \quad (5.16)$$

but, because of the cavity equations, each of the summand is at sight positive (and zero if  $j$  is the “arg-second” index at all times of the period).

## Chapter 6

# Statistical analysis of the Cavity Algorithm

Thanks to the convergence of the bias fields to an optimal assignment, it is possible to address a set of questions of primary importance in the discussion of a practical algorithm. First we present a numerical analysis of the convergence time distribution and its scaling behaviour with the size of the instances. The problem of algebraic tail in the solution times, is then faced suggesting a possible workaround.

### 6.1 Convergence time analysis

Helped by the existence of a very effective algorithm for solving the Assignment Problem, the Hungarian Algorithm, even in the “basic” implementation of the cavity algorithm, like e.g., in a framework of [2], where we do not have neither a certificate, nor even a halting condition, it makes sense to study the “optimistic lower-bound” to the solution time, i.e., the iteration time at which for the first instant the optimal solution is identified. More or less optimistic criteria can be defined, and have been studied, as described in greater detail below, while the numerical analysis of the convergence time is shown in figure 6.1. The comparison with the optimal matching  $\pi$  is done via the argmax functions over the bias fields  $\bar{k}_j(t)$  and  $\bar{l}_i(t)$ :

$$\begin{cases} \bar{l}_i(t) = \arg \max_j (-\varepsilon_{ij} - h_{j \rightarrow i}^{(t-1)}) \\ \bar{k}_j(t) = \arg \max_i (-\varepsilon_{ij} - g_{i \rightarrow j}^{(t)}) \end{cases} \quad (6.1)$$

Three criteria have been used in order to define a “solution time”:

1. A first threshold  $t_0$  is placed in the first time after which the argmax functions over the bias fields coincide with the optimal solution for a number of iterations of order  $\mathcal{O}(N)$ ,

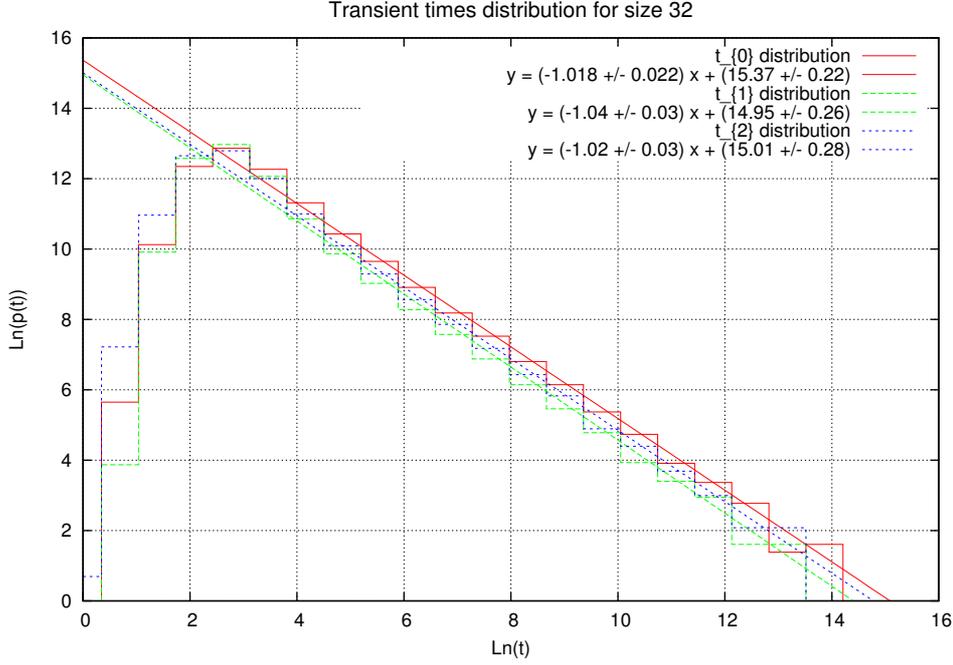


Figure 6.1: Solving time distribution for an ensemble of instances at size 32. On the x-axis there is the natural logarithm of solving times, while on the y-axis is represented the natural logarithm of the number of instances fallen in the interval of the histogram.

with  $N$  the size of the cost matrix (i.e., it finds the solution in a *persistent* way)

$$t_0 = \min_t \left\{ t \in \mathbb{N} : \forall \tau \leq N, \forall i, j, \bar{l}_i(t + \tau) = \pi_i \wedge \bar{k}_j(t + \tau) = \pi_j^{-1} \right\} \quad (6.2)$$

2. A weaker form selects the first time in which the condition is satisfied, even if not in persistent way

$$t_1 = \min_t \left\{ t \in \mathbb{N} : \forall i, j, \bar{l}_i(t) = \pi_i \wedge \bar{k}_j(t) = \pi_j^{-1} \right\} \quad (6.3)$$

3. Another still weaker form allows some a number of order 1 of nodes constraints to be unsatisfied (2, in our numerics)

$$t_2 = \min_t \left\{ t \in \mathbb{N} : \forall \tau \leq N, \text{for at least } N - 2 \text{ indices } i \quad \bar{l}_i(t + \tau) = \pi_i \right. \\ \left. \wedge \text{for at least } N - 2 \text{ indices } j \quad \bar{k}_j(t + \tau) = \pi_j^{-1} \right\} \quad (6.4)$$

Remark that these weak criteria are very “generous”: for example, allowing for a few errors corresponds to the assumption that one could recover the true solution from an almost-good

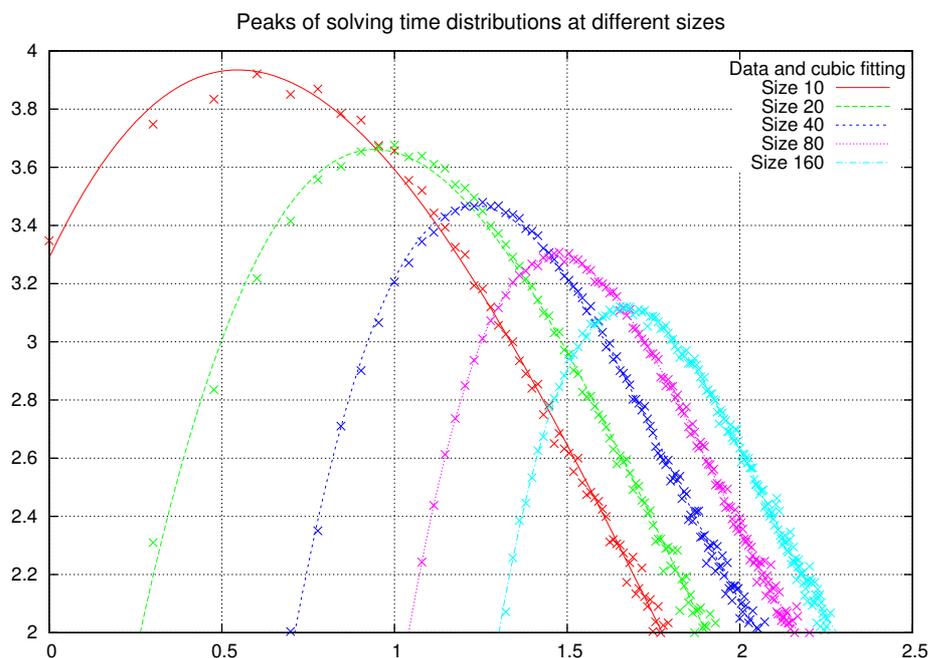


Figure 6.2: Distribution of solving times in a log-log representation. Only peaks are shown.

one with some polynomial procedure, still to identify. Still, no one of the generous criteria we used is significantly better than the original one, and in particular all of them show intractable non-integrable algebraic tails in the distribution of the solution times – our estimate for the exponent is  $-1.018 \pm 0.022$ , calculated with the proper prescription of statistical data analysis:

$$\begin{cases} \alpha = 1 + n \left( \sum_i \log \frac{x_i}{x_0} \right)^{-1} \\ \sigma = \frac{1 + \alpha}{\sqrt{n}} \end{cases} \quad (6.5)$$

where  $x_0$  represents the cutoff from which the tail is considered,  $n$  the size of the sample, and  $\sigma$  the variance or error. The “intuition” on this exponent is on the fact that, as in the estimates of the proof, the slow instances are the ones in which a parameter  $\Delta$ , combination of our weights, and thus in  $\mathbb{R}$ , and positive by definition, is very near to zero. In this case, the solution times could slow up to times of order  $\Delta^{-1}$ . If the distribution of the  $\Delta$  has finite support at  $\Delta = 0$  (as it clearly does, cfr. the numerics below), one would thus experience an exponent exactly  $-1$ .

A comparison at different sizes is shown in figure 6.2 alongside with a tempted finite size scaling analysis in figure 6.3.

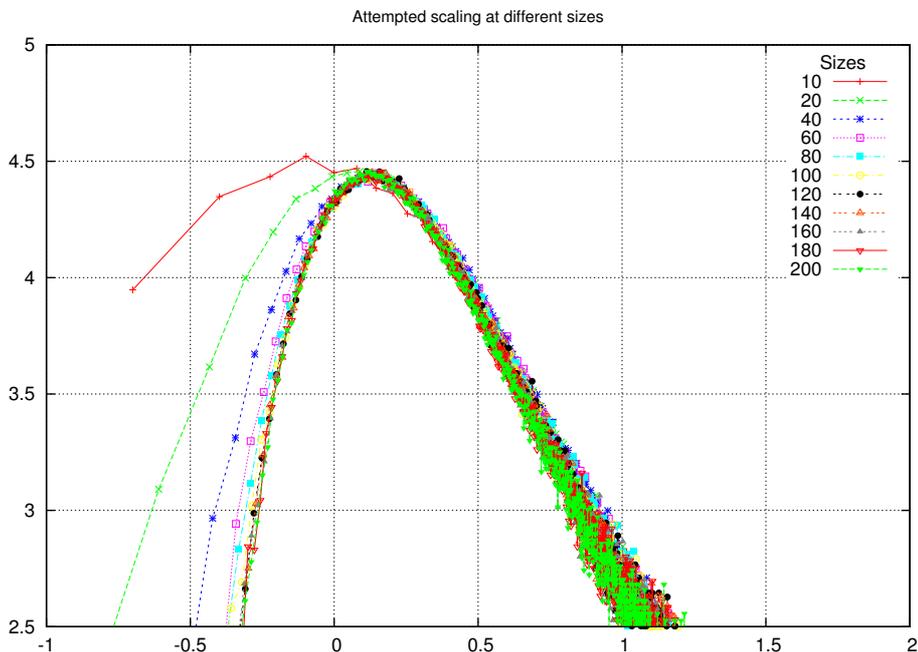


Figure 6.3: Here is a tempted collapse curve for the previous distributions for the following transformation:  $(t; p(t)) \mapsto (\log_{10} t - 0.7 \log_{10} N; \log_{10} p(t) + 0.6 \log_{10} N)$ .

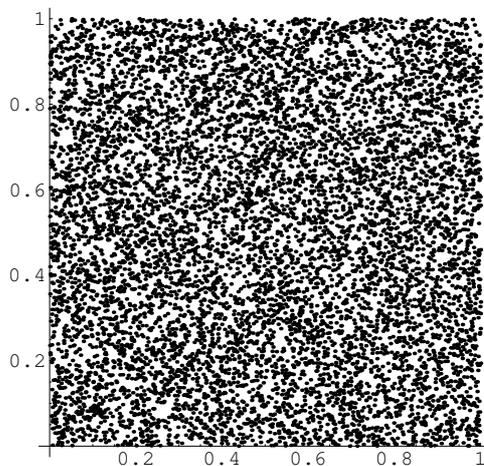
These preliminary considerations are useful to stress that even if a convergence proof exists, nonetheless projection on minimal cost configuration happens in a very awkward way, even in the most favourable case like those in the weaker criteria. Letting alone the criteria with *a priori* knowledge of the solution, surely it is important to have an optimality certificate, that does not require hard test on the stationary phase phenomena. Thus the certificate presented in section 5.2 is the key for the a practical algorithm, but, in order to address the effectiveness, we should first understand in more details which are the causes at the root of slow instances.

## 6.2 Statistical properties of convergence parameters

The distribution of the drifts  $\Delta$  has been investigated numerically. As the costs at given instance are some random process, although correlated, and each cost is the sum of  $N$  real numbers, we could expect that single consecutive spacings (such as  $\Delta$  is) are random in some way analogous to a Poisson Process (although on long sequences of costs we would not expect such an idea to be valid). Indeed, collected data for  $10^5$  random instances, of sizes  $N = \{32, 64, 128, 256\}$  (cfr. figure 6.4), show quite evidently a distribution of drifts  $\Delta$  at size  $N$  compatible with an exponential of

width  $2/N^2$ . We do not have however analytical arguments for justifying the exact value of 2, although maybe arguments in the fashion of [21] could succeed in this.

The distribution of the second spacing, called  $\Delta_{12}$  in the discussions of section 5.2, is however not well fitted by a single exponential, and seems to be spectrally richer. Nonetheless, it seems quite well verified that the pairs  $(\Delta, \Delta_{12})$  are almost decorrelated. At support of this claim, we show, for a list of about  $10^5$  instances of size 256, the plot of the pairs  $(i, j)$  such that for the given seed  $\Delta$  is the  $i$ -th of the sorted list, and  $\Delta_{12}$  is the  $j$ -th (actually, with normalized entries), and we interpret the results from the fact that no special structure seems to arise (correlation or anticorrelation would concentrate the points on one or the other of the two diagonals).



The distribution of periods in the drift cycle, i.e., the parameter  $\ell(\pi, \pi')$  realizing the minimum drift  $\Delta$ , in the notations of section 5.2, or equivalently the number of iterations  $T$  in the recipe for the certificate of equation (5.8), have been studied at various sizes ( $N = \{32, 64, 128, 256\}$ ), and a scaling analysis has been performed, assuming a Gaussian form like

$$\text{prob}(T; N) \propto \sqrt{\frac{1}{N}} \exp\left(-\frac{T^2}{\alpha N}\right) \quad \text{for } T \text{ integer } \geq 2. \quad (6.6)$$

with  $\alpha$  some constant not determined. The collapse of the curves is quite good (with numerical estimate of  $\alpha = 1.40 \pm 0.05$ ), and is shown in figure 6.5.

The guess of a Gaussian fit was also suggested by a naïve argument: at the end of the cavity algorithm, the set of “speaking” edges consists of a Hungarian tree (it is in general a Hungarian Forest at the end of the traditional Hungarian Algorithm, but our prescription produces a “condensation” of the components). The drift cycle is all contained in the tree, except for a single edge not in the matching. If we also include this edge, we have a “Hungarian unicyclic”. Assuming (in a totally unjustified way) an uniform distribution over the possible unicyclics on

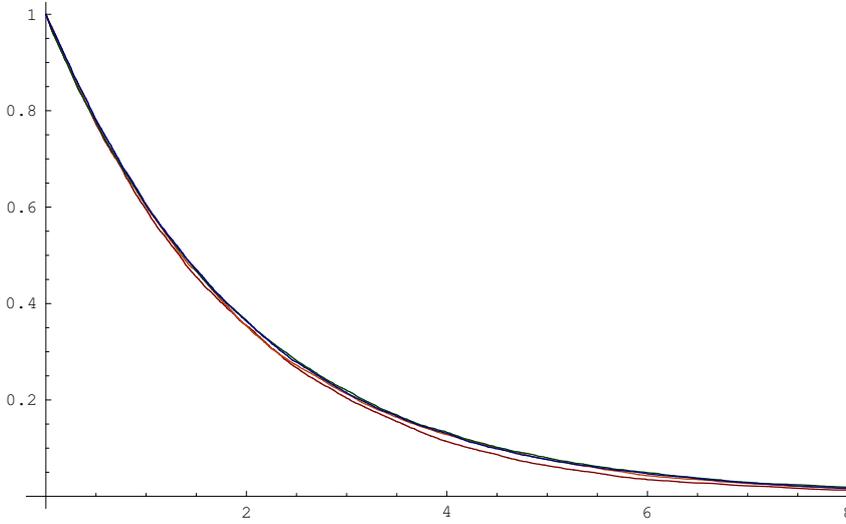


Figure 6.4: Cumulant distribution of the quantities  $N^2\Delta$  for random instances at size  $N$  (i.e.,  $f(x)$  is the probability that  $N^2\Delta > x$ ). Sizes are  $N = \{32, 64, 128, 256\}$  (with colours respectively: red, orange, green, blue). The fit with an exponential of width 2 has not been reported, because indistinguishable from the numerical data.

the complete bipartite graph, we obtain that relative probabilities for cycles of length  $2T$  go like

$$\text{prob}(T; N) \propto \frac{N(N-1)\cdots(N-T+1)}{N^T} \simeq e^{-\frac{1}{N}-\frac{2}{N}-\cdots-\frac{T-1}{N}} \simeq \exp\left(-\frac{T(T-1)}{2N}\right) \quad (6.7)$$

which appears to be qualitatively correct, although it does not estimate the proper value of  $\alpha$ .

### 6.3 Fast solution of slow instances: the fork-after-warning procedure

As explained, the dynamics of bias fields is led by the passing of messages through some alternating cycles between matchings in the bipartite graph. Every cycle has a proper weight that determines its likely to be an active channel for the messages, this weight being the alternating sum of edge weights in one or in another matching. The cavity equations, through the local iterative map, select those cycles whose total drift, i.e., weight divided by the cycle length, is minimal. Very small drifts thus, cause a slowing down of the convergence process, but there is also another cause, not so much with respect to the selection of the minimal matching, but rather for the selection of the first excited cycle, being their difference  $\Delta_{12}$  in the driving force toward equilibrium. That should not mislead: the selection of the minimal matching, causes the

system to evolve towards configurations with the optimal matching, but, for the certification, i.e., for reaching the proper stationary phase, also the second matching should be fixed by the dynamics. It is thus not surprising that instances could exist with very long certificate time, even if, maybe, the spread between the ground state and the first excited matching is not so small. Such considerations could be explained through fig. 6.6.

We recognize a dense ellipse of “typical” cases, with some correlation, and three “tails”: one shows strong correlation: we had a long time “because”  $\Delta$  or  $\Delta_{12}$  (resp. if red or green) were anomalously small; one is almost horizontal (but only green) and corresponds to parameters  $\Delta_{12}$  anomalously small, which did not cause the instance to be slow; one is almost vertical, corresponds to slow instances, which were not anomalous in respect to  $\Delta$  or to  $\Delta_{12}$ , and is potentially dangerous, as, if it turns out that some of these instances were slow although *both*  $\Delta$  and  $\Delta_{12}$  were typical, we would have failed in detecting all the possible causes of slow instances. For this reason, on the bottom of the figure, we plot a subset of the red (resp. green) points, selecting only the ones in which the parameter  $\Delta$  is smaller than  $\Delta_{12}$  (or vice-versa). The vertical tail has disappeared, so that we can guess that all slow instances were indeed caused by an anomalously small value of  $\min(\Delta, \Delta_{12})$ .

We can now suggest a quite simple idea with relevant consequences: what if a better inspection of the transient phase, say, of the first  $\mathcal{O}(N)$  iterations or even less, almost always succeed in identifying the presence of a cycle with drift anomalously small, and did not find a large fraction of spurious irrelevant small-drift cycles?

In this case, we would have “morally” identified the reason for the future slowing of the algorithm, within a typical solution time, and we could adopt a whatever reasoning for circumvent this to happen. The conceptually more economic way is to “fork” the process: take a whatever edge of the dangerous cycle, say the one connecting row  $i$  to column  $j$ , and change its weight to, e.g., a quite large value (so that one restricts to configurations  $\pi$  in which  $\pi(i) \neq j$ ). Then solve the resulting instance, say finding a minimum energy  $E_1$ , most probably in a “typical” time. Then, for the same edge, shift up of a large amount the weight of all the other entries  $(i, j')$  with  $j' \neq j$  (so that one restricts to the complementary set of configurations  $\pi$  in which  $\pi(i) = j$ ). Then solve also this resulting instance, say finding a minimum energy  $E_2$ , again most probably in a “typical” time. The configuration corresponding to the minimum energy among  $E_1$  and  $E_2$  is thus the global minimum of the original instance, and has been found within three typical times. This would kill any algebraic tail, and cause an almost-gaussian distribution of solution times, analogously to the Hungarian Algorithm.

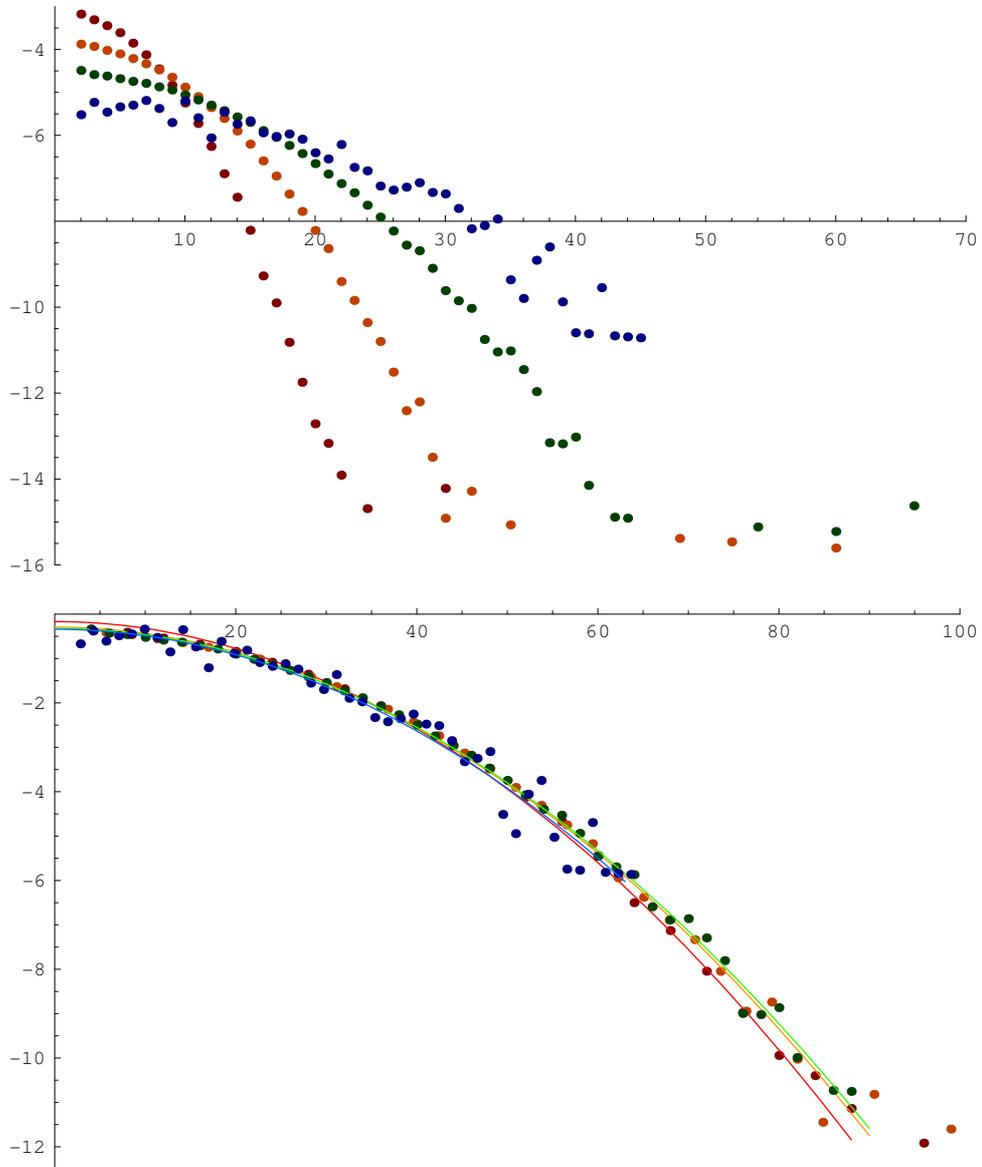


Figure 6.5: Top: distribution of the periods for random instances of sizes  $N = \{32, 64, 128, 256\}$  (colours respectively: red, orange, green, blue); on  $x$  axes: the period in units of interactions, on  $y$  axes: logarithm of the fraction of events. Bottom: collapse of the curves, and fit of the single-size data with a Gaussian. Values on  $y$  axes have been shifted of  $\log_2(N/2)$ , while values on  $x$  axes have been scaled of factors  $\sqrt{512/N}$ .

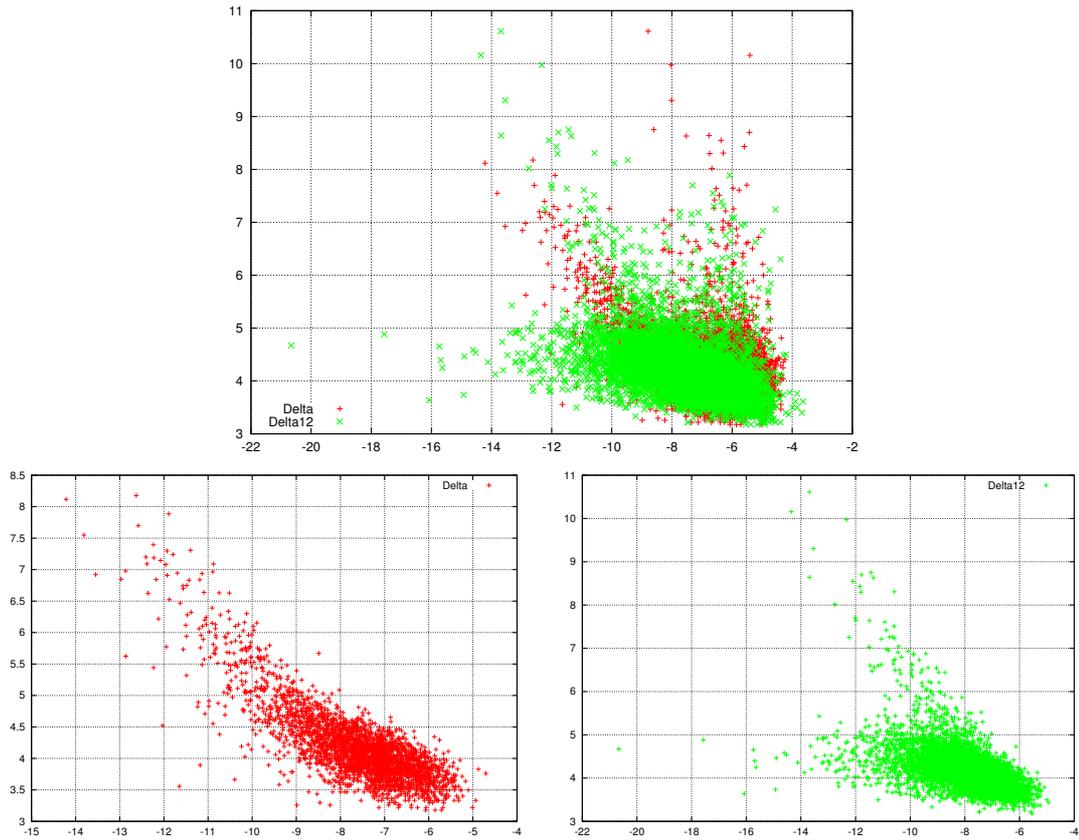


Figure 6.6: Plot, in log-log scale, of the number of iterations required in our “basic” algorithm in order to reach a certificate (i.e., in our algorithm, without the technique of “fork-after-warning” described below). Times are the  $y$  coordinate of each point. On the  $x$  axes is reported the logarithm of the parameter  $\Delta$  (red point), or of the parameter  $\Delta_{12}$  (green point).



# Conclusion and perspective

As was pointed out in some recent papers [22] the Cavity Equations (i.e., the autoconsistencies equations for the cavity fields introduced in chapter 3) are powerful tools to solve some problems of Combinatorial Optimization. But, in spite of the fact they help us to solve some problems also in the hard regions, not much is known about the existence of a solution and an eventual convergence towards this solution. Only for a few set of problems we know that a solution of the Cavity Equations exists and can be reached. Among this problems there are all the ones that can be expressed as an Hamiltonian with a tree-like Factor Graph.

In this thesis we studied how the Cavity Equations works on the assignment problem that is a polynomial problem, i.e., it has been showed [6] an algorithm able to solve all the instances in a time that grows polynomially with the problem size. This problem can not be described in terms of a Hamiltonian with a tree-like Factor Graph, so we had no guarantee of existence of a fixed point or convergence to the solution. The Assignment problem is interesting for its practical applications, but also for its theoretical properties. In fact applying the Cavity Equations as recursive equations on the fields which live on the directed edges of the factor graph it was observed that after a transient time a set of fields begins to drift towards  $+\infty$  and another set drift towards  $-\infty$ . The set of fields that goes negatively to infinity results to be the fields on the site of the factor graph that should be set to the configuration. This fact, up to what we know, is the only one case were a similar behaviour happens. As we showed the presence of loops (normally dangerous for the search of solution via Cavity Methods) here happens to play an important role in determining the specific behaviour of the evolution of the Cavity Fields.

An extensive analysis of the average and typical times involved in the dynamics of the algorithm on a random set of instances was done so to give us a deeper comprehension of the phenomenon and of its finite size-scaling behaviour. The problem in the infinite size limit result to have an infinite transient time.

We observed that a mechanical implementation of the equations is not an algorithm. As a matter of fact, it can not output the solution in any way, also if it “found” the right answer and the mean time needed to find this solution is infinite (due to rare instances of very slow convergence time), in other words there was not a recipe to stop the algorithm whenever it finds

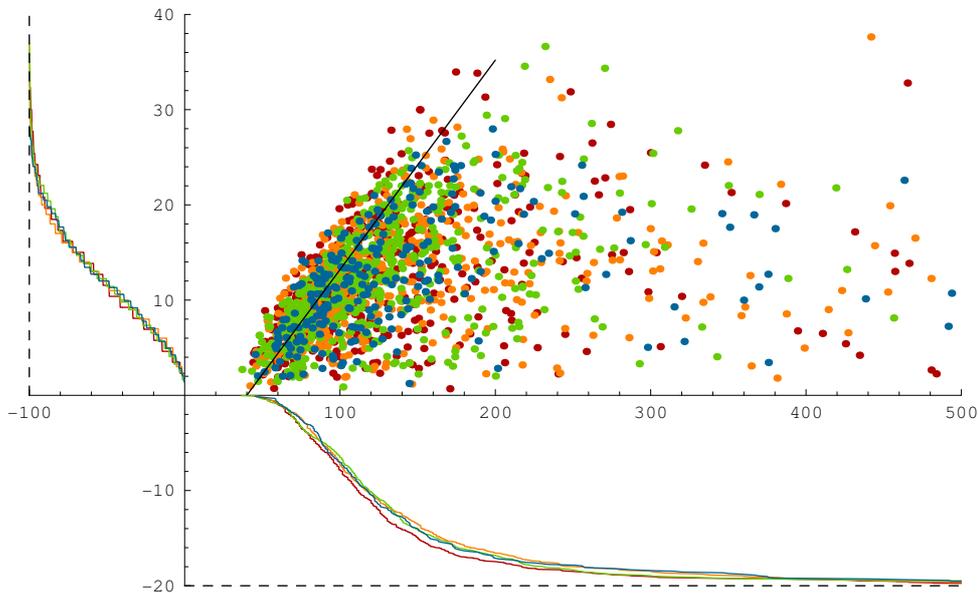


Figure 6.7: In figure you can find a comparison of the solving times between Hungarian Algorithm and the cavity one. Each point represents an instance (different colours are user for different sizes:  $N = \{32, 64, 128, 256\}$  correspond to red, orange, green and blue points), whose abscissa value correspond to the computing time with the Cavity Algorithm, while in its ordinate value is the Hungarian Algorithm computing time. Times are scaled, both in  $x$  and  $y$  directions, by a factor  $\propto N^3$ . Sub-figures in quadrant II and IV corresponds to Hungarian and Cavity computing time cumulant distributions. The algebraic tail in bare Cavity Algorithm is evident, while Hungarian times are Gaussianly concentrated.

the solution, because there was not a way to recognize that the one found was the solution. The time needed to solve an instance was finite but arbitrarily long, so that the average time resulted to be infinite on the space of random instances in which each entry of the cost matrix is a random number with a given distribution, independent on each entry, not concentrated and not null on zero).

One of our main contribution is to have written a working algorithm for the Assignment, with Cavity Methods, meaning an algorithm that gives always a solution and do it in a finite. In fact we found an halting condition, i.e., the algorithm is now able to say if a feasible solution is a solution and we showed that this happens always (the algorithm is always able to find this certificate). We found how to speed up the rare very-slow instances (the ones responsible for the infinite mean time), so to make the solution time finite on average and not only for each instance.

So, after to have given a physical formulation of the problem (in terms of the Hamiltonian on the factor graph and of the gauge fields) we found the mechanism governing the evolution for the Assignment Problem, we found a Cavity Algorithm working on this problem, able to find the solution in a finite time and we extensively studied the behaviours of all the quantity related to the fields dynamics.

We were interested on the theoretical properties of the problem in its formulation as a disordered system. But the advantage (in technological terms) that the Cavity Algorithm presents on the classical ones is to be more easy to implement (it's a sequence of few and very easy operations) so that it's possible to think to an hardware implementation of a Cavity Algorithm.

What would be interesting to determine is if there is the possibility, by using some tricks to write an algorithm competitive with the famous one written by Kuhn (this is a difficult task because the existing algorithms use some strong properties of the matching among bipartite set). The use of these properties makes the algorithm very efficient but more involute that the cavity one.

One important open point remains: if and how it is possible to export the tools we founded for the Assignment problem to other problems. We do not know any problem whose dynamics exhibits the same specific properties of the Assignment (like the drifting fields), but it would be an interesting task to force another problem to have the same objects that generate this peculiar dynamics so to obtain the same behaviour and to make it possible an efficient solution via the Cavity Equations.

Looking at figure 6.7, one could grasp an overall comparison with the exact Hungarian Algorithm. Even if it seems clear that the Hungarian Algorithm has globally better performance, it should be also noted that the Cavity Algorithm has two features of great interest:

- It seems better suited for a hardware implementation, either parallel, or not, for the Hungarian Algorithm, being rooted in graph theory, is relatively a complex algorithm, requiring a set of nontrivial computing structures. In this comparison, the architecture of the Cavity Algorithm, instead, is much simpler, involving, in its core, just additions and maximum operation over matrix elements.
- Second, it should be noted that the Hungarian Algorithm computes a dynamics in the matching space with no guarantee of closeness to the best solution, thus, in realtime application can perform quite badly. On the converse, the global updating procedure of the Cavity Algorithm, let hope to derive simple recipes to extract from transient time configurations a good, but maybe suboptimal, candidate assignment.



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