Optimization in mean field models

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1 Introduction

The non-rigorous cavity method of statistical mechanics, originally developed in the study of spin glasses and other disordered systems, has led to a number of purely mathematical predictions. Several of them can be found in the remarkable book [17] by Marc Mézard, Giorgio Parisi and Miguel Angel Virasoro. Establishing these predictions rigorously remains a challenge to probability theory. Important achievements in this direction are David Aldous' proof of the $\zeta(2)$ limit in the assignment problem [4], Michel Talagrand's proof of the correctness of the Parisi solution of the Sherrington-Kirkpatrick model [9, 24], and the algorithmic and theoretical results on phase transitions in constraint satisfaction problems [1, 2, 18].

One of the areas where the statistical mechanics view has produced a number of challenging conjectures is optimization in mean field models of distance. In the simplest of these models there are n vertices labeled $1, \ldots, n$. Each pair of vertices is connected by an edge, and the edges (i, j) are assigned i. i. d. random costs $X_{i,j}$ (sometimes thought of as representing distance) from a given distribution μ on the nonnegative real numbers. In general one is interested in the large n ("thermodynamical") limit of the cost of a solution to a combinatorial optimization problem.

I will describe a mathematically rigorous method whose underlying idea resembles the cavity method. Several new results have been established with this method, some of which were anticipated by the cavity approach. For instance we have established the "mean field limit" for the traveling salesman problem, conjectured in [11, 14, 15].

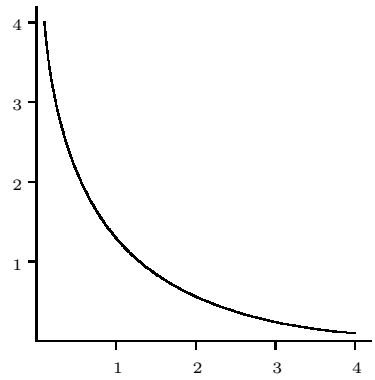

Figure 1: The curve $(1+\frac{x}{2})e^{-x}+(1+\frac{y}{2})e^{-y}=1$.

Let L_n be the cost of the minimum traveling salesman tour, that is, the minimum sum of the edge costs of a cycle that visits each vertex exactly once. Further, we define the number $L^\star \approx 2.04$ by

$$L^\star = \frac{1}{2}\int_0^\infty y\,dx, \tag{1}$$

where $y(x)$ is the positive solution to the equation

$$\left(1+\frac{x}{2}\right)e^{-x}+\left(1+\frac{y}{2}\right)e^{-y}=1, \tag{2}$$

see Figure 1.

Theorem 1.1. *If the distribution μ satisfies*

$$\frac{P(X_{i,j}<t)}{t}\to 1, \quad \textit{as } t\to 0+, \tag{3}$$

then

$$L_n \xrightarrow{\mathrm{p}} L^\star, \quad \textit{as } n\to\infty. \tag{4}$$

This problem has been studied extensively, theoretically as well as by computer simulation [4, 5, 10, 11, 14, 15, 17]. Until now the most precise estimate of $\lim_{n\to\infty} L_n$ was obtained with the cavity method. The value 2.0415 is given in [11]. This value is consistent with the less precise estimates

obtained by simulation. Using equation (1) we have found, to 26 decimal places,

$$L^\star = 2.04154818641213241804549016\ldots$$

After a discussion of Theorem 1.1, G. Parisi (in personal communication) has shown that the analytic characterization of $L^\star$ obtained in equations (6) and (9) of [11] is equivalent to (1). In fact this was the first proof that equation (6) of [11] (with $r = 0$) has a unique solution. This brings us to the satisfactory conclusion that the cavity result is exact.

2 Temperature and annealing

An interesting question is how our method relates to the statistical mechanics approach. The details of this relationship are not yet clear, and it remains to be seen whether similar methods can put other cavity results on firm mathematical ground.

In the language of statistical mechanics, the cost of an optimization problem corresponds to the *hamiltonian* $H(\sigma)$ of a physical system. The system is supposed to act somewhat as if it tried to find a state σ that minimizes this quantity. The tendency to minimize the hamiltonian is governed by the temperature T. This is reflected by the *Gibbs measure*, in which the probability of finding the system in a particular state σ is proportional to

$$\exp(-H(\sigma)/T).$$

In the limit $T \to 0$, the Gibbs measure concentrates at the *ground state*, in other words the state that minimizes H. Physically, the meaning of temperature is intuitively clear, but in the mathematical setting, it is not obvious why one should introduce this parameter. An idea which is present both in the cavity approach and in the *simulated annealing* paradigm of computer science is to introduce the parameter T and then to let $T \to 0$, thereby forcing the system to converge to its ground state.

The mean field models that we study are roughly of the following type: There is a set of random variables $X_1, \ldots, X_N$ (the edge costs). A state σ is a subset of $\{1, \ldots, N\}$ (a set of edges), and the hamiltonian is given by

$$H(\sigma) = \sum_{i \in \sigma} X_i.$$

If the variables X_i are exponential of rates r_i as in [6], then we can think of them as generated from an underlying set $Y_1, \ldots, Y_N$ of rate 1 exponential variables by $X_i = Y_i/r_i$. Then the Gibbs measure becomes

$$P(\sigma) \propto \exp\left(-\sum_{i\in\sigma} \frac{Y_i}{T \cdot r_i}\right).$$

If we allow the rates r_i to vary, there is no point in introducing the parameter T. Rescaling all the rates will give the same effect as changing the temperature, which means that we can put $T = 1$ without loss of generality.

Conversely, we can regard each rate r_i as a local temperature parameter associated to the variable Y_i. As in [6], we associate a parameter (called the *weight*) to each vertex rather than to the edges. Following the cavity method, we relax the optimization problem by introducing an extra vertex. Then, realizing that the weight of this vertex plays the role of a local temperature parameter, we apply the annealing trick and force the system back to its original state by letting the weight of the extra vertex tend to zero. It may come as a surprise that this gives us information about the distribution of $\min_\sigma H(\sigma)$, since at first it looks like we only get the original problem back.

Our approach is based on an exact solution of a certain class of "friendly" problems. The first example of this kind was the formula conjectured by G. Parisi for the cost A_n of the bipartite assignment problem with exponential edge costs [22]. This formula,

$$E(A_n) = 1 + \frac{1}{4} + \frac{1}{9} + \cdots + \frac{1}{n^2}, \tag{5}$$

was proved in [12, 19, 20]. We introduce a random model that we call the *friendly model*. In this model there is a large class of linear programming problems that have similar exact solutions. In particular we have established an analogue of (5) for the complete graph. For a suitable linear relaxation of the perfect matching problem, the expectation of the cost C_n of the minimum solution is given by the alternating sum

$$E(C_n) = 1 - \frac{1}{4} + \frac{1}{9} - \cdots + \frac{(-1)^{n-1}}{n^2}. \tag{6}$$

3 The random flow problem

3.1 The friendly model

In Section 3.2 we define a class of optimization problems whose feasible solutions include loops and multiple edges. Here we introduce a random model that contains such edges. This model is designed to allow for exact identities like (5) and (6). We will refer to it as the *friendly model*. There are n vertices $v_1, \ldots, v_n$. Each vertex v_i has a positive real *weight* γ_i. For each i and j there is a potentially infinite set of edges connecting v_i and v_j. If $i \neq j$, these edges have costs that are determined by the times of the events in a Poisson process of rate $\gamma_i\gamma_j$. If $i = j$, there is a set of loops at this vertex, and their costs are given by a Poisson process of rate $\gamma_i^2/2$. All these Poisson processes are independent.

This model has a certain self-similarity. If we group the vertices into sets and regard the edges as connecting these sets instead of the individual vertices, we obtain a structure that behaves in the same way as the original model. For a set S of vertices, let

$$\gamma_S = \sum_{i \in S} \gamma_i.$$

If S and T are disjoint, then the edges that connect S and T have costs given by a Poisson process of rate $\gamma_S\gamma_T$, while the costs of the edges that have both their endpoints in S are given by a process of rate $\gamma_S^2/2$.

3.2 Flow problems

If we are given a set $V = \{v_1, \ldots, v_n\}$ of n vertices, and guaranteed the existence of arbitrarily many edges between each pair of vertices (including loops), we can define a certain type of optimization problem that we call *flow problem*. We let each vertex v_i have a nonnegative integer *capacity* c_i. Let E denote the set of edges. For each $e \in E$, let $X_e \geq 0$ be the cost of e. For $e \in E$ and $v \in V$ we use the notation $\langle e, v \rangle$ for the number of times that e is connected to v. In other words

$$\langle e, v \rangle = \begin{cases} 2, & \text{if } e \text{ is a loop at } v, \\ 1, & \text{if } e \text{ connects } v \text{ to another vertex,} \\ 0, & \text{otherwise.} \end{cases}$$

For a nonnegative integer k, the flow problem asks for the vector $\sigma : E \to \mathbb{R}$ that minimizes

$$\sum_{e \in E} \sigma(e) X_e, \tag{7}$$

subject to the constraints

- For each $e \in E$, $0 \leq \sigma(e) \leq 1$,
- σ respects the capacity constraints at each vertex, that is, for each i,

$$\sum_{e \in E} \langle e, v_i \rangle \, \sigma(e) \leq c_i, \tag{8}$$

- The total size of σ is (at least) $k/2$:

$$\sum_{e \in E} \sigma(e) \geq k/2. \tag{9}$$

  Since the edge costs X_e are all nonnegative, we can obviously replace the inequality in (9) by equality.

There exist feasible solutions if and only if $0 \leq k \leq \sum_{1 \leq i \leq n} c_i$. A vector σ that satisfies the constraints (that is, a feasible solution) will be called a *flow*. If equality holds in (9), σ is called a k-flow. The left-hand side of (8) is called the *degree* of v_i with respect to σ. If equality holds in (8), we say that v_i has *full degree* in σ.

In the *generic* case, when there are no linear relations between the edge costs, there is a unique minimum k-flow for every k. In the friendly model, genericity holds with probability 1. In the following, we sometimes assume genericity without explicitly stating this assumption. We denote the minimum k-flow by σ_k (without assuming genericity, this notation would be ambiguous). The cost of σ_k is denoted C_k, and the degree of v_i in σ_k is denoted $\delta_k(i)$.

4 The annealing method

Suppose that we are given a random flow problem in the friendly model, as described in Sections 3.1 and 3.2. This means that we have specified the number n, the weights $\gamma_1, \ldots, \gamma_n$ and the capacities $c_1, \ldots, c_n$. We also fix

a positive integer $k \leq \sum_{1 \leq i \leq n} c_i$. As was explained informally in Section 2, we introduce an extra vertex v_{n+1} of weight γ_{n+1} and capacity 1. In the following, quantities referring to this extended graph will be denoted with a superscript $(n+1)$.

For the moment, we fix a vertex v_i, $1 \leq i \leq n$. Since $c_{n+1} = 1$, only one edge between v_i and v_{n+1} is relevant to the flow problem. We denote this edge by e_i and note that the cost $X_{i,n+1}$ of e_i has exponential distribution of rate $\gamma_i \gamma_{n+1}$, in other words, the density is

$$\gamma_i \gamma_{n+1} e^{-\gamma_i \gamma_{n+1} t}$$

for $t \geq 0$. We are interested in the expected value of the coefficient $\sigma_k^{(n+1)}(e_i)$ of e_i in the minimum k-flow in the extended graph, as a function of γ_{n+1}.

Let us for the moment condition on the costs of all other edges. We let $f(x)$ denote the cost of the minimum k-flow on the extended graph given that $X_{i,n+1} = x$. We have

$$Ef(X_{i,n+1}) = \gamma_i \gamma_{n+1} \int_0^\infty e^{-\gamma_i \gamma_{n+1} x} f(x)\, dx.$$

Moreover, the coefficient $\sigma_k^{(n+1)}(e_i)$ is the derivative of $f(x)$ at $x = X_{i,n+1}$. Here we disregard the fact that there may be a finite number of points where f is non-differentiable. The following calculations by partial integration only require f to be continuous. We have

$$E\left[\sigma_k^{(n+1)}(e_i)\right] = \int_0^\infty \gamma_i \gamma_{n+1} e^{-\gamma_i \gamma_{n+1} x} f'(x)\, dx.$$

By partial integration, this is equal to

$$\gamma_i \gamma_{n+1} \left[\int_0^\infty \gamma_i \gamma_{n+1} e^{-\gamma_i \gamma_{n+1} x} f(x)\, dx - f(0) \right] = \gamma_i \gamma_{n+1} \left[EC_k^{(n+1)} - \left(C_k^{(n+1)} | X_{i,n+1} = 0 \right) \right]. \quad (10)$$

Notice that we are still conditioning on all edge costs except $X_{i,n+1}$. In (10), we therefore regard $(C_k^{(n+1)} | X_{i,n+1} = 0)$ as a non-random quantity.

We let the superscript $(\hat{i})$ denote a flow problem where the capacity c_i is decreased by 1 (assuming that originally this capacity was nonzero). Since one possibility of obtaining a k-flow in the extended graph is to use the edge

e_i together with the minimum $(k-2)$-flow given this decreased capacity of v_i, we have

$$\left(C_k^{(n+1)} | X_{i,n+1} = 0\right) \leq C_{k-2}^{(\hat{i})}.$$

If we regard the edge costs as generated from an underlying set of rate 1 variables as described in Section 2, then we can let $\gamma_{n+1} \to 0$ for a fixed point in the probability space. It is clear that, pointwise,

$$C_k^{(n+1)} \to C_k \quad \text{and} \quad \left(C_k^{(n+1)} | X_{i,n+1} = 0\right) \to C_{k-2}^{(\hat{i})}.$$

By the principle of dominated convergence we conclude from (10) that as $\gamma_{n+1} \to 0$,

$$\frac{E\left[\sigma_k^{(n+1)}(e_i)\right]}{\gamma_{n+1}} \to \gamma_i \left(EC_k - EC_{k-2}^{(\hat{i})}\right). \tag{11}$$

So far we have conditioned on all edge costs except the cost $X_{i,n+1}$ of e_i. At this point it is clear that (11) must hold also if we interpret the expectations as averages over all edge costs.

In fact there are methods that allow us to compute the expected degree of a vertex in the minimum flow. In particular, this allows us to compute

$$\lim_{\gamma_{n+1} \to 0} \frac{1}{\gamma_{n+1}} \cdot \sum_{i=1}^{n} E\left[\sigma_k^{(n+1)}(e_i)\right],$$

which by (11) is equal to

$$\left(\sum_{i=1}^{n} \gamma_i\right) \cdot EC_k - \sum_{i=1}^{n} \gamma_i EC_{k-2}^{(\hat{i})}. \tag{12}$$

A convenient way to state this equation is

$$EC_k = \frac{1}{\gamma_1 + \cdots + \gamma_n} \cdot \lim_{\gamma_{n+1} \to 0} \frac{E\left[\delta_k^{(n+1)}(n+1)\right]}{\gamma_{n+1}} + EC_{k-2}^{(\hat{i})}, \tag{13}$$

where in the last term, $EC_{k-2}^{(\hat{i})}$ is interpreted as an average over a random choice of i, taken with probabilities proportional to the weights, in other words, the probability of choosing a particular i is

$$\frac{\gamma_i}{\gamma_1 + \cdots + \gamma_n}.$$

Provided that we can compute the expected degree of a vertex in the solution to a random flow problem in the friendly model, equation (13) allows us to compute EC_k recursively by first computing $EC_{k-2}^{(\hat{i})}$ for $1 \leq i \leq n$.

5 The average degree of a vertex in the minimum k-flow

Suppose that the weights and capacities are given, and let $K = \sum_{1 \leq i \leq n} c_i$. Recall that $\delta_0, \ldots, \delta_K$ are the degree vectors for the flows $\sigma_0, \ldots, \sigma_K$. In this section we define another random process based on the weights and capacities. This process was introduced by Marshall Buck, Clara Chan, and David Robbins [6], and we refer to it as the Buck-Chan-Robbins urn process. It turns out that several quantities associated to the random flow problem have counterparts in the urn process. Virtually all our "exact" results for the flow problem state that some random variable defined in terms of the flow problem has the same expectation as a corresponding random variable defined in terms of the urn process. In this section we define the one-dimensional version of the urn process and show how $E\delta_k(i)$ can be interpreted in terms of this process.

An urn contains balls labeled $1, \ldots, n$, one ball corresponding to each vertex in the graph. The balls have weights $\gamma_1, \ldots, \gamma_n$. Each time a ball is drawn from the urn, it is chosen among the balls in the urn with probabilities proportional to the weights. The capacities $c_1, \ldots, c_n$ serve as *replacement protocol*: The balls that are drawn from the urn are put back into the urn as long as they have not been drawn a number of times equal to their capacity. When ball i has been drawn c_i times, it is removed.

The results in this section can be stated for a discrete time version of this process, where balls are simply drawn one at a time from the urn. However, it is convenient to introduce a continuous time version of the process, where the balls are drawn at random times independently of each other. This is achieved by letting ball i be drawn from the urn at times determined by a rate γ_i Poisson process. As soon as ball i has been drawn c_i times, it is removed.

We record the outcome of the urn process by letting $D_k(i)$ be the number of times that ball i occurs among the first k times that a ball is drawn from the urn. Notice that the distribution of $D_k(i)$ depends on the weights as

well as the capacities, but that it is independent of whether we regard the process as discrete or continuous time. Our method is based on the following proposition:

Proposition 5.1.

$$E\delta_k(i) = ED_k(i).$$

Let T_k be the time at which the k:th ball is drawn in the urn process.

Lemma 5.2.

$$\lim_{\gamma_{n+1}\to 0} \frac{E\left[\delta_k^{(n+1)}(n+1)\right]}{\gamma_{n+1}} = ET_k.$$

Proof. By Proposition 5.1, we have

$$E\left[\delta_k^{(n+1)}(n+1)\right] = ED_k^{(n+1)}(n+1).$$

We have to prove the identity

$$\lim_{\gamma_{n+1}\to 0} \frac{ED_k^{(n+1)}(n+1)}{\gamma_{n+1}} = ET_k. \tag{14}$$

This identity concerns the urn process only. We have

$$ED_k^{(n+1)}(n+1) = P(t < T_k),$$

where t is the time at which ball $n+1$ is drawn. This is equal to

$$E\left[1 - \exp(-\gamma_{n+1}T_k)\right]. \tag{15}$$

The left-hand side of (14) is the (right) derivative of (15) as $\gamma_{n+1} \to 0+$. By differentiating, this is equal to

$$T_k \cdot \exp(-\gamma_{n+1}T_k) \to T_k,$$

as $\gamma_{n+1} \to 0+$. □

6 The two-dimensional urn process

Suppose that the number n of vertices, the weights γ_i and the capacities c_i are given. We use the results of Sections 4 and 5 to obtain a "formula" for EC_k. This formula is expressed in terms of a two-dimensional version of the urn process. In this version, there are two independent urn processes on the vertices. The two processes take place in two independent directions along the x- and y-axes in a two-dimensional time plane. For each vertex v_i, we let $P_i(x)$ be the number of times that the vertex v_i has been drawn in the first process (the x-process) up to time x. Similarly, let $Q_i(y)$ be the number of times that v_i has been drawn in the second urn process up to time y. We define the rank of the process for the single vertex v_i at time (x, y) by

$$\mathrm{Rank}_i(x, y) = \min(P_i(x), c_i) + \min(P_i(x) + Q_i(y), c_i). \tag{16}$$

The total rank of the process is defined by

$$\mathrm{Rank}(x, y) = \sum_{i=1}^{n} \mathrm{Rank}_i(x, y).$$

We let $R_k = R_k(c, \gamma)$ be the region in the positive quadrant of the x-y-plane for which $\mathrm{Rank}(x, y) < k$. The following theorem gives an exact characterization of EC_k.

Theorem 6.1.

$$EC_k = E\left[\mathrm{area}(R_k)\right].$$

Proof. This follows inductively from (13) and Proposition 5.1. Suppose by induction that $EC_{k-2}^{(\hat{i})} = E\left(\mathrm{area}(R_{k-2}^{(\hat{i})})\right)$ for $1 \le i \le n$. Then by (13) and Lemma 5.2,

$$EC_k = \frac{1}{\gamma_1 + \cdots + \gamma_n} \cdot ET_k + E\left[\mathrm{area}(R_{k-2}^{(\hat{i})})\right]. \tag{17}$$

We have to show that the right-hand side of (17) is equal to $E\left[\mathrm{area}(R_k)\right]$. Therefore consider the urn process. Let x_0 be the time at which the first ball is drawn in the x-process. Then the expected area of the part of R_k that lies in the strip $0 < x < x_0$ is

$$\frac{ET_k}{\gamma_1 + \cdots + \gamma_n}$$

which is the first term in the right-hand side of (17).

The probability that the first ball to be drawn is the one labeled i is

$$\frac{\gamma_i}{\gamma_1 + \cdots + \gamma_n}.$$

If this happens, then the expected area of the remaining part of R_k (for which $x > x_0$) is equal to

$$E\left[\text{area}(R_{k-2}^{(\hat{i})})\right],$$

which is the second term of (17). □

If all vertices have capacity 1 and $k = n$, the flow problem is an LP-relaxation of the perfect matching problem. It is easy to show that in this case, Theorem 6.1 specializes to (6).

7 Estimate of the size of the region R_k

Using standard techniques of probability theory, one can obtain estimates of the expected area of R_k, and thereby of EC_k.

Suppose that n and k are given. Let $R^\star$ be the non-random region given by

$$E\left(\text{Rank}(x, y)\right) \leq k.$$

One can establish the following upper bound on the difference between the area of $R^\star$ and the expected area of R:

Theorem 7.1. *If for every i, $\gamma_i = 1$ and $c_i \leq 2$, then*

$$\left|E\left(\text{area}(R)\right) - \text{area}(R^\star)\right| = O\left(\frac{(\log n)^{3/2}}{n^{1/2}}\right).$$

In the case that all vertices have capacity 2, and $k = 2n$, the region $R^\star$ is precisely the region under the curve in Figure 1.

8 The TSP versus the 2-factor problem

In [8], Alan Frieze studied the relation between the 2-factor problem and the TSP on the complete graph K_n with uniform $[0, 1]$ edge costs. With our

notation, L_n is the length of the minimum tour and Z_n is the length of the minimum 2-factor. Frieze proved that

$$L_n - Z_n = o(1) \quad \text{whp as } n \to \infty. \tag{18}$$

When the edge costs are known, Z_n is computable in polynomial time. In [8], Frieze showed that with high probability, the minimum 2-factor can be "patched" to a tour at small extra cost, and that this can be done in polynomial time. Hence a polynomial time algorithm will produce a tour that with high probability is not much worse than the minimum tour. Using Fireze's method, we can prove the following theorem:

Theorem 8.1. *In the friendly model with weights $\gamma_i = 1$,*

$$E\,|L_n - L^\star| = O\left(\frac{(\log\log n)^{1/2}}{(\log n)^{1/4}}\right).$$

In particular, as n tends to infinity, $EL_n \to L^\star$ and $L_n \xrightarrow{\mathrm{p}} L^\star$.

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