Local entropy as a measure for sampling solutions in Constraint Satisfaction Problems

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We introduce a novel Entropy-driven Monte Carlo (EdMC) strategy to efficiently sample solutions of random Constraint Satisfaction Problems (CSPs). First, we extend a recent result that, using a large-deviation analysis, shows that the geometry of the space of solutions of the Binary Perceptron Learning Problem (a prototypical CSP), contains regions of very high-density of solutions. Despite being sub-dominant, these regions can be found by optimizing a local entropy measure. Building on these results, we construct a fast solver that relies exclusively on a local entropy estimate, and can be applied to general CSPs. We describe its performance not only for the Perceptron Learning Problem but also for the random K-Satisfiability Problem (another prototypical CSP with a radically different structure), and show numerically that a simple zero-temperature Metropolis search in the smooth local entropy landscape can reach sub-dominant clusters of optimal solutions in a small number of steps, while standard Simulated Annealing either requires extremely long cooling procedures or just fails. We also discuss how the EdMC can heuristically be made even more efficient for the cases we studied.

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I. INTRODUCTION

Markov Chain Monte Carlo (MCMC) algorithms for combinatorial optimization problems are designed to converge to a stationary distribution $\pi$ that is a monotone decreasing function of the objective function one needs to minimize. A fictitious temperature is usually introduced to make the distribution more and more focused on the optima. Depending on the form of the stationary distribution (i.e. on the temperature) the sampling process can converge fast or it can get trapped in local minima. There is typically a tradeoff between optimality of the sampled solutions and the form of $\pi$: smooth and close to uniform distributions are the easiest to sample but the sampled configuration are most often far from optimal. On the contrary hard to sample distributions are characterized by a so called glassy landscape where the number of metastable minima that can trap the MCMC and brake ergodicity are typically exponentially numerous [1, 2].

Random constraint satisfaction problems (CSPs) offer an ideal framework for understanding these type of questions in that they allow to analyze the geometry of the space solutions of hard to sample problems and at the same time design and test novel algorithms [3]. In many random CSPs, the computational hardness is associated to the existence of optimal and metastable states that are grouped into different clusters of nearby solutions with different sizes and properties. Finer geometrical properties of the space of solutions have been investigated in the literature [4–6], but a general scenario has yet to be established.

Large deviation analysis allows to describe in some detail the structures of such clusters, ranging from the dominant clusters (those in which one would fall by choosing uniformly at random a solution) to the subdominant ones. Note that in general, algorithms are by no means bounded to sample solutions uniformly at random.

Very recently it has been shown [7] that problems that were believed to be intractable due to their glassy nature, namely the learning problems in neural networks with discrete synaptic weights, possess in fact a richer structure of the space of solutions than what is suggested by the standard equilibrium analysis. As it turns out, there exist sub-dominant and extremely dense clusters of solutions that can be analytically unveiled by defining a probabilistic weight based on the local entropy, i.e. on the number of solutions within a given radius from a reference solution. Despite being sub-dominant, these states turn out to be accessible by extremely simple heuristic algorithms.
Here, we move forward and study the same structures without enforcing the constraint that the reference configuration is itself a solution. This apparent simplification actually requires higher levels of replica-symmetry breaking in the analysis. The resulting measure defines an objective function, namely the local entropy, that we then use to devise a novel MCMC, which we call Entropy-driven Monte Carlo (EdMC). When applied to the binary perceptron learning problem, EdMC yields algorithmic results that are in very good agreement with the theoretical computations, and by far outperform standard Simulated Annealing in a direct comparison.

We also applied this approach to the $K$-SAT problem, showing that even when some of the computations can not be carried out exactly the practical performance is indeed very good even in hard regions. Further heuristic algorithmic improvements are also discussed.

Here, we focus on the representative case of zero temperature and Hamming distance, but the technique could be easily extended to go beyond these simple assumptions.

The rest of the paper is organized as follows: in Sec. I A we present the results of the analysis of the sub-dominant clusters of solutions and define the novel EdMC algorithm, in Sec. II we report extensive numerical results, comparing EdMC to the theoretical results and to standard Simulated Annealing, while in Sec. III we discuss our findings. Two Appendices follow the main text: in the first, Appendix A, we provide details about the Belief Propagation algorithm; in the second, Appendix B, we report a detailed self-contained description of the analytical computations.

A. Sub-dominant clusters analysis and Entropy-driven Monte Carlo

In most random combinatorial optimization problems the so called dominating states of the equilibrium Gibbs measure at zero temperature (the ground states) are not relevant in the analysis of practical optimization algorithm and their dynamics. The algorithmically accessible states are typically sub-dominant states characterized by a high internal entropy [8]. The structure of such sub-dominant states can be investigated by means of the Replica Method or the Cavity Method, at least in the average case.

The approach we will present in the following extends our recent findings in the discrete Perceptron Learning Problem [7], where we carried out a large deviations analysis by introducing a reweighting of the solutions by the local entropy, i.e. by the number of other
solutions surrounding a given one. We show that even if we remove the explicit constraint that the reference configuration is a solution, optimizing the local entropy has approximately the same effect with high probability: in other words we find that if we can estimate the local entropy for any given configuration, and then seek the configuration for which it is maximum, in all likelihood we will end up in a solution.

This naturally raises the possibility to translate such theoretical predictions into a general practical solver, because even though computing the local entropy may be more difficult than computing the energy, the resulting landscape may be radically different. A simple and direct way to show that this is the case is to compare two MCMC implementations, one optimizing the energy and one optimizing the local entropy (we call the latter Entropy-driven Monte Carlo, or EdMC). Indeed, the local entropy landscape proves to be much smoother, allowing to reach ground states inaccessible to the energetic MCMC.

1. Large deviations analysis of CSPs

A generic Constraint Satisfaction Problem (CSP) can be defined in terms of configurations of \( N \) variables \( x_i \in X_i \), subject to \( M \) constraints \( \psi_\mu : D_\mu \rightarrow \{0,1\} \). Each constraint \( \mu \) involves a subset \( \partial_\mu \) of the variables, which we collectively represent as \( x_{\partial_\mu} = \{ x_i : i \in \partial_\mu \} \in D_\mu \), and we define \( \psi_\mu (x_{\partial_\mu}) = 1 \) if the constraint is satisfied, 0 otherwise. For concreteness, let us focus on the case of binary spin variables \( X_i = X = \{-1,+1\} \), the generalization to multi-valued variables being straightforward [9]. We may define an energy function of the system simply as the number of violated constraints, namely:

\[
H(x) = \sum_\mu E_\mu (x_{\partial_\mu}) = \sum_\mu (1 - \psi_\mu (x_{\partial_\mu}))
\] (1)

A solution of a CSP is then a zero-energy configuration. The standard zero-temperature Gibbs measure for CSPs, which we will call equilibrium measure, assumes uniform weight over the space of solutions and it is the one associated to the partition function

\[
\mathcal{N} = \lim_{\beta \rightarrow \infty} \sum_x e^{-\beta H(x)} = \sum_x \prod_\mu \psi_\mu (x_{\partial_\mu})
\] (2)

which just counts the solutions.
Suppose now one wants to analyze the local structure of the solution space by counting the number of solution vectors $x$ around a given planted vector $\tilde{x}$. To this end, we define the local free entropy, as a function of the planted configuration, as:

$$F(\tilde{x}, \gamma) = \frac{1}{N} \log \mathcal{N}(\tilde{x}, \gamma)$$

(3)

where

$$\mathcal{N}(\tilde{x}, \gamma) = \sum_x \prod_{\mu} \psi_{\mu}(x_{\partial \mu}) e^{\gamma x \cdot \tilde{x}}$$

(4)

counts all solutions to the CSP with a weight that depends on the distance from $\tilde{x}$ and is modulated by the parameter $\gamma$. Solving a CSP amounts to finding a solution vector $\tilde{x}^*$ such that $H(\tilde{x}^*) = 0$: we shall show below that this can be achieved by optimizing the cost function $F(\tilde{x}, \gamma)$ over $\tilde{x}$, which naturally guides the system in a region with a high density of solutions. In order to determine $F(\tilde{x}, \gamma)$, one needs to study a slightly different system then the one defined by $H(x)$, in which the variables $x_i$'s are coupled to some external fields $\gamma \tilde{x}_i$, with $\tilde{x}_i \in \{-1, +1\}$ and $\gamma \in \mathbb{R}$ is the coupling strength. Thus the directions of the external fields $\tilde{x}_i$'s are considered as external control variables. The parameter $\gamma$ sets the magnitude of the external fields, and in the limit of large $N$ it effectively fixes the Hamming distance $d$ of the solutions $x$ from $\tilde{x}$. The local free entropy $F(\tilde{x}, \gamma)$ is then obtained as the zero-temperature limit of the free energy of the system described by $H(x; \tilde{x})$, and can be computed by Belief Propagation (see Sec. I A 4 and Appendix A).

We then study a system defined by the following free energy:

$$\mathcal{F}(\gamma, y) = -\frac{1}{Ny} \log \left( \sum_{\tilde{x}} e^{yNF(\tilde{x}, \gamma)} \right)$$

(5)

where $y$ has formally the role of an inverse temperature and $-F(\tilde{x}, \gamma)$ has formally the role of an energy. Throughout the paper the term temperature will always refer to $y^{-1}$ except where otherwise stated. In the limit of large $y$, this system is dominated by the ground states $\tilde{x}^*$ for which the local free entropy is maximum; if the number of such ground states is not exponentially large in $N$, the local entropy can then be recovered by computing the Legendre transform

$$\mathcal{F}(\gamma, \infty) = -\mathcal{F}(\gamma, \infty) - \gamma S$$

(6)

where $S$ is the typical value of the overlap $\frac{x \cdot \tilde{x}^*}{N}$. This quantity thus allows us to compute

$$e^{N \mathcal{F}(\gamma, \infty)} = \mathcal{N}(\tilde{x}^*, \gamma) = \sum_x \prod_{\mu} \psi_{\mu}(x_{\partial \mu}) \delta( NS - x \cdot \tilde{x}^*)$$

(7)
i.e. to count the number of solutions at normalized Hamming distance $d = \frac{1-S}{2}$ from the ground states $\tilde{x}^*$ (note that the soft constraint of eq. 4 is equivalent to a hard constraint in the limit of large $N$, but that the opposite is not true in general — see Sec. B1 for more details on this point).

Informally speaking, if the distance $d$ is small enough (i.e. at large $\gamma$), then $\tilde{x}^*$ is going to be roughly at the center of a dense cluster of solutions, if such cluster exists, which means that it is likely going to be a solution itself (indeed, that is surely the case when $d = 0$). Furthermore, because of the reweighting term, these dense solution regions will typically have different statistical properties with respect to the set of thermodynamically locally stable states. We therefore refer to these solutions as sub-dominant clusters, since they are not normally part of the equilibrium description. However, we have reasons to believe that these kind of sub-dominant clusters play a crucial role in the algorithmic properties of practical learning problems in CSPs: the analysis of the local free entropy $F(\tilde{x}^*, \gamma)$ in the case of the binary perceptron learning problem (see below) has shown that indeed such sub-dominant ultra-dense regions exist at least up to a critical value of the parameter $\alpha = \frac{M}{N}$, that these kind of solutions exhibit different properties with respect to typical equilibrium solutions, and that heuristic solvers typically find a solution in such regions \cite{7}.

2. Two prototypical CSPs

In this paper we consider two prototypical CSPs, which are both computationally hard but have very different characteristics and structure. The first one — the main focus of this paper — is the binary Perceptron Learning Problem, a fully connected problem that originally motivated our investigation. The second is an example of a general diluted problem, the Random $K$-SAT, which has a long tradition in the Statistical Mechanics of Optimization Problems.

a. Binary perceptron  Let us consider the problem of classifying $M = \alpha N$ input patterns $\xi^\mu \in \{-1, +1\}^N$, that is associating to each of them a prescribed output $\sigma^\mu \in \{-1, +1\}$. The perceptron is defined as a simple linear threshold unit that implements the mapping $\tau(x, \xi) = \text{sign}(x \cdot \xi)$, with $x$ representing the vector of synaptic weights. In what follows we will consider the classification problem, which consists in finding a vector $x^*$ that correctly classifies all inputs, i.e. $\tau(x^*, \xi^\mu) = \sigma^\mu$, $\mu \in \{1, ..., M\}$, given a set of random i.i.d. unbiased
\{\xi^\mu, \sigma^\mu\}. We will focus on the case of spin-like weights, i.e. \( x \in \{-1, +1\} \) (the generalization to more states does not pose significant additional difficulties). The corresponding energy function is the sum of wrongly classified patterns, namely:

\[
H_{\text{perc}}(x) = \sum_{\mu} \Theta(-\sigma^\mu \tau(x, \xi^\mu))
\]

where \( \Theta(\cdot) \) is the Heaviside step function. This problem has been extensively analyzed in the limit of large \( N \) by means of Replica \([10, 11]\) and Cavity \([12]\) methods, finding that in the typical case there is an exponential (in \( N \)) number of solutions up to a critical capacity \( \alpha_c = 0.833 \), above which no solution typically exists. Despite the exponential number of solutions, the energetic landscape is riddled with local minima, and energetic local search algorithms are typically ineffective at finding them for any \( \alpha \) \([13–15]\). Moreover typical solutions are known to be isolated \([15]\).

**b. \( K\)-SAT** The satisfiability problem, in its ‘random \( K\)-SAT’ instantiation, consists in finding an assignment for \( N \) truth values that satisfies \( M = \alpha N \) random logical clauses, each one involving exactly \( K \) different variables. Let us then consider \( N \) Boolean variables \( \{t_i \in \{0, 1\}\} \), with the common identification \( \{0 \rightarrow \text{FALSE}, 1 \rightarrow \text{TRUE}\} \). A given clause \( \mu \) is the logical OR of its variables, whose indices are \( i^\mu_1, \ldots, i^\mu_K \), and which can appear negated. Let us work in a spin representation \( x_i = 2t_i - 1 \) and introduce the couplings \( J^\mu_{i_r} \in \{-1, +1\} \), where \( J^\mu_{i_r} = 1 \) if the variable \( x_{i^\mu_r} \) appears negated in clause \( \mu \), and \( J^\mu_{i_r} = -1 \) otherwise. The graph structure is random, in that each clause involves \( K \) variables extracted uniformly at random, and the couplings are also unbiased i.i.d. random binary variables. With these definitions, the solutions to a \( K\)-SAT problem are the zero energy configurations of the following Hamiltonian:

\[
H_{\text{SAT}} = 2 \sum_{\mu=1}^{M} \prod_{k=1}^{K} \left( 1 + \frac{J^\mu_{i_k} x_{i^\mu_k}}{2} \right)
\]

which counts the number of violated clauses.

Random \( K\)-SAT has been central in the development of the statistical mechanical approach to CSPs. For more details, we refer the reader to comprehensive reviews \([2, 16]\). Here we just point out that, when varying the number of constraints per variable \( \alpha \), the problem undergoes a sequence of phase transitions, related to the fragmentation of the phase space in a huge number of disconnected clusters of solutions. This rich phenomenology, observed well below the UNSAT threshold (above which no solution typically exists at large \( N \)), can
be analyzed by the cavity method in the framework of 1-step Replica Symmetry Breaking (1-RSB), and is reflected in the exponential slowing down of greedy algorithms as well as sampling strategies.

### 3. 1-Step Replica-Symmetry-Broken solution in the binary perceptron

The existence of dense sub-dominant regions of solutions with radically different properties than those described by the usual equilibrium analysis was first discovered for the perceptron learning problem in [7], as a result of extensive numerical simulations and of the study of a free energy function very similar to eq. (5).

The free energy used in [7] differs from the one of eq. (5) because in the latter we do not impose any constraint on the reference configurations $\tilde{x}$. In [7], we analyzed the free energy using the Replica Method at the level of a Replica Symmetric (RS) solution, and found that there was a maximum value of $y$ for which the external entropy was non-negative. The external entropy is the logarithm of the number of configurations $\tilde{x}^\ast$ divided by $N$, and should not take finite negative values: when it does, it means that there is a problem in the RS assumption. Therefore, in that analysis, we used the value $y^\ast$ that led to a zero complexity.

We repeated the RS computation for the unconstrained version, eq. (5), and found that as $\alpha$ increases the results become patently unphysical. For example, the RS solution at $y = y^\ast$ would predict a positive local entropy even beyond the critical value $\alpha_c$. Therefore, the RS assumption needs to be abandoned and at least a 1-step of Replica Symmetry Breaking (1-RSB) must be studied. Specifically, we assumed that RSB occurred at the level of the $\tilde{x}$ variables, while we kept the RS Ansatz for the $x$ variables, and computed the result in the limit $y \to \infty$. This appears as a geometrically consistent assumption, in that the clusters we are analyzing are dense and we do not expect any internal fragmentation of their geometrical structure. All the details of the calculation are in the Appendix B. The result is a system of 8 coupled equations, with $\alpha$ and $S$ as control parameters (using $S$ as control parameter instead of its conjugate $\gamma$ which was used in eq. 5 is advantageous for the theoretical analysis at high $\alpha$, see below).

Solving these equations still yields a negative external entropy for all values of $\alpha$ and $S$, and studying the finite $y$ case is numerically much more challenging in this case, to
the point of being presently unfeasible. However, the magnitude of the external entropy is greatly reduced with respect to the analogous RS solution at $y \to \infty$; furthermore, its value tends to zero when $S \to 1$, and all the other unphysical results of the RS solution were fixed at this step of RSB. Additionally, the qualitative behavior of the solution is the same as for the constrained RS version of [7]. Finally, simulation results, where available, are in remarkable agreement with the predictions of this computation (see below, Sec. II A 1). We therefore speculate that this solution is a reasonable approximation to the correct solution at $y \to \infty$.

In particular, these qualitative facts hold (see Fig. 1):

1. For all $\alpha$ below the critical value $\alpha_c = 0.83$, the local entropy in the region of $S \to 1$ tends to the curve corresponding to $\alpha = 0$, implying that for small enough distances the region around the ground states $\tilde{x}^*$ is extremely dense (almost all points are solutions).

2. There is a transition at $\alpha_U \simeq 0.77$ after which the local entropy curves are no longer monotonic; in fact, we observe the appearance of a gap in $S$ where the system of equations has no solution. We speculatively interpret this fact as signaling a transition between two regimes: one for low $\alpha$ in which the ultra-dense regions are immersed in a huge connected structure, and one at high $\alpha$ in which the structure of the sub-dominant solutions fragments into separate regions.

Two additional results are worth noting about the properties of the reference configurations $\tilde{x}$ (see Appendix B 3 for the complete details):

1. In the limit $y \to \infty$, the the local entropy takes exactly the same value as for the constrained case in which the $\tilde{x}$ are required to be solutions, and the same is true for the parameters that are common to both cases. The external entropy, however, is different. This is true both in the RS and the 1-RSB scenario.

2. For the unconstrained case, we can compute the probability that the reference configuration $\tilde{x}$ makes an error on any one of the patterns (see Fig. 2). It turns out that this probability is a decreasing function of $S$ (going exponentially to 0 as $S \to 1$) and an increasing function of $\alpha$. For low values of $\alpha$, this probability is extremely low, such that at finite values of $N$ the probability that $\tilde{x}$ is a solution to the full pattern set is almost 1.
Figure 1. **A.** Local entropy vs overlap $S$, at various values of $\alpha$. All curves tend to the $\alpha = 0$ case for sufficiently high $S$. For $\alpha \gtrsim 0.77$, a gap appears, i.e. a region of $S$ where no solution to the saddle point equations exists. For $\alpha \gtrsim 0.79$, some parts of the curve have negative entropy (dashed). All curves reach a plateau for sufficiently low values of $S$ where the local entropy becomes equal to the equilibrium entropy (not shown). **B.** Relationship between the overlap $S$ and its conjugate parameter, the external field $\gamma$. Up to $\alpha \lesssim 0.75$, the relationship is monotonic and the convexity does not change for all values of $S$; up to $\alpha \lesssim 0.77$, a solution exists for all $S$ but the relationship is no longer monotonic, implying that there are regions of $S$ that cannot be reached by using $\gamma$ as an external control parameter. The gap in the solutions that appears after $\alpha \gtrsim 0.77$ is clearly signaled by the fact that $\gamma$ reaches 0; below $\alpha_c = 0.83$, a second branch of the solution always reappears at sufficiently high $S$, starting from $\gamma = 0$.

Figure 2. **A.** Probability of a classification error by the optimal reference configuration $\tilde{x}$, for various values of $\alpha$, as a function of $S$. The dashed parts of the curves correspond to the parts with negative local entropy (cf. Fig. 1); the curves have a gap above $\alpha \gtrsim 0.77$. **B.** Same as panel A, but in logarithmic scale on the $y$ axis, which shows that all curves tend to zero errors for $S \to 1$. 
4. EdMC: Local entropy as an alternative objective function in optimization

The case of the binary perceptron suggests that it is possible to exploit the results of the sub-dominant analysis and devise a simple and fairly general scheme for solving CSPs in a very efficient and controlled way.

For the binary perceptron, Fig. 1B shows that up to $\alpha \lesssim 0.75$ we can use $\gamma$ as a control parameter to determine $S$, while Fig. 2 shows that a solution to the learning problem can be found by maximizing the local free entropy $F(\tilde{x}, \gamma)$ (eq. (3)) as a function of $\tilde{x}$ at sufficiently large $\gamma$.

The reason to follow this strategy, as opposed to directly trying to minimize the energy $H_0(\tilde{x})$ (eq. (1)), is that it turns out that the landscape of the two objective functions is radically different: while the energy landscape can be riddled with local minima that trap local search algorithms, the local entropy landscape is much smoother. Therefore, a simple Monte Carlo algorithm on the local free entropy, or “Entropy-driven Monte Carlo” (EdMC) for short, is able to effectively find solutions that are very hard to find for energy-based simulated annealing.

Furthermore, the behavior of this algorithm can — at least in principle — be described in the typical case with the tools of Statistical Mechanics, to the contrary of what is currently possible for the other efficient solvers, which all, to some extent, resort to heuristics (e.g. decimation, soft decimation a.k.a. reinforcement, etc.).

Indeed, the main practical difficulty in implementing the EdMC algorithm sketched above is estimating the local free entropy $F(\tilde{x}, \gamma)$. We use the Belief Propagation (BP) algorithm for this, a cavity method algorithm that computes the answer in the context of the Bethe Approximation. The BP algorithm is briefly explained in the Appendix A, where we also reported the specific BP equations used for the particular CSPs that we studied in this paper.

More specifically: $\tilde{x}$ is initialized at random; at each step $F(\tilde{x}, \gamma)$ is computed by the BP algorithm; random local updates (spin flips) of $\tilde{x}$ are accepted or rejected using a standard Metropolis rule at fixed temperature $y^{-1}$. In practice, we found that in many regimes it suffices to use the simple greedy strategy of a zero temperature Monte Carlo ($y = \infty$). From a practical standpoint, it seems more important instead to start from a relatively low $\gamma$ and increase it gradually, as one would do in a classical annealing procedure. We call such
procedure ‘scoping’, as it progressively narrows the focus of the local entropy computation to smaller and smaller regions. The reason to adopt such a strategy is easily understood by looking at the theoretical error probability curves in Fig. 2.

II. EDMC RESULTS

In what follows, we will describe EdMC in more detail for the two prototypical examples introduced in Sec. I A 2.

A. Perceptron

1. Comparison with theoretical results

We tested the theoretical results of Sec. I A 3 by running EdMC on many samples at 
\( N = 201 \) and \( \alpha = 0.6 \), at various values of \( \gamma \) (we used \( \gamma = \tanh^{-1}(p) \), varying \( p \in [0.4, 0.9] \) in steps of 0.1). In this case, since we sought the optimum value of the free local entropy \( F(\hat{x}, \gamma) \) at each \( \gamma \), we did not stop the algorithm when a solution was found. We ran the algorithm both directly at \( y = \infty \) and using a cooling procedure, in which \( y \) was initialized at 5 and increased by a factor of 1.01 for every 10 accepted moves. The search was stopped after \( 5N \) consecutive rejected moves. For each sample and each polarization level, we recorded the value of the overlap \( S \), of the local entropy \( S \) (see eq. 6 above and eqs. (A11) and (A12) in the Appendix A) and of the error probability per pattern. Then, we binned the results over the values of \( S \), using bins of width 0.005, and averaged the results of the local entropy and the error rate in each bin. Fig. 3 shows that both values are in reasonable agreement with the theoretical curve: the qualitative behavior is the same (in particular: the error rate goes to zero at \( S \to 1 \) and the entropy is positive until \( S = 1 \), confirming the existence of dense clusters) and the more accurate version is closer to the theoretical values. The remaining discrepancy could be ascribed to several factors: 1) finite size effects, since \( N \) is rather small 2) inaccuracy of the Monte Carlo sampling, which would be fixed by lowering the cooling rate 3) inaccuracy of the theoretical curve due to RSB effects, since we know that our solution is only an approximation.

Note that, with these settings, the average number of errors per pattern set is almost always less than 2 for all points plotted in Fig. 3A. Also note that, for all values of \( S \), the
Figure 3. *EdMC vs theoretical results.* A. Probability of error on a pattern (cf. Fig. 2) B. Local entropy (cf. Fig. 1A). See text for details on the procedure. For the version with cooling, 700 pattern sets were tested for each value of $\gamma$. For the $y = \infty$ version, 2000 samples were used. Error bars represent standard deviation estimates of the mean values.

mode and the median of the error distribution is at 0, and that the average is computed from the tails of the distribution (which explains the noise in the graphs). Finally note that, for all samples, points corresponding to 0 errors were found during the Monte Carlo procedure.

2. *Comparison with standard Simulated Annealing*

We tested our method with various problem sizes $N$ and different values of $\alpha$, and compared its performance with a standard MCMC. The most remarkable feature of EdMC is its ability to retrieve a solution at zero temperature in a relative small number of steps. We found that zero temperature MCMC (Glauber dynamics) immediately gets trapped in local minima at zero temperature, even at small $N$. In order to find a solution with MCMC we used a simulated annealing (SA) approach, with initial inverse temperature $y_0 = 1$, and we increased $y$ by a factor $f_y$ for every $10^3$ accepted moves. The factor $f_y$ is a cooling rate parameter that we optimized for each problem instance (see below). Fig. 4 shows a comparison between a typical trajectory of SA versus EdMC on the very same instance (EdMC is run at $y = \infty$ with $\gamma = \tanh^{-1}(0.6)$): at first glance, it exemplifies the typical difference in the average number of steps required to reach a solution between SA and EdMC, which is of 4 or 5 orders of magnitude for small $N$. Also note the smoothness of the EdMC trajectory in contrast to SA: the local entropy landscape is far smoother and ensures a rapid convergence to the region with highest density of solutions.
Figure 4. Perceptron Learning Problem, $N = 801$, $\alpha = 0.3$. Typical trajectories of standard Simulated Annealing on Hamiltonian (8) (red curve, right) and Entropy-driven Monte Carlo (blue curve, left). Notice the logarithmic scale in the $x$ axis. EdMC is run at 0 temperature with fixed $\gamma = \tanh^{-1}(0.6)$, SA is started at $y_0 = 1$ and run with a cooling rate of $f_y = 1.001$ for each $10^3$ accepted moves, to ensure convergence to a solution.

We studied the scaling properties of EdMC in contrast to SA, at $\alpha = 0.3$ and $\alpha = 0.6$, varying $N$ between 201 and 1601 and measuring the number of iterations needed to reach a solution to the learning problem.

For the SA tests, we used the following procedure: for each instance of the problem, we tried to find a solution at some value of the cooling rate $f_y$; after $10^5 N$ consecutive rejected moves, we started over with a reduced $f_y$, and repeated this until a solution was eventually found. The values of $f_y$ that we used were $\{1.1, 1.05, 1.02, 1.01, 1.005, 1.002, 1.001, 1.0005, 1.0001\}$. This allowed us to measure the least number of iterations required by SA to solve the problem (we only report the number of iterations for the last attempted value of $f_y$).

At $\alpha = 0.3$, all tested instances were solved, up to $N = 1601$. At $\alpha = 0.6$, however, this procedure failed to achieve 100% success rate even for $N = 201$ in reasonable times; at $N = 401$, the success rate was 0% even with $f_y = 1.0001$; at $N = 1601$, using $f_y = 1.0001$ did not seem to yield better results than $f_y = 1.1$. Therefore, no data is available for SA at $\alpha = 0.6$.

For the EdMC tests, we used the following procedure: we started the algorithm at $\gamma =$
Figure 5. Perceptron Learning Problem. Number of iterations required to reach 0 energy in log-log scale, as a function of the problem size $N$. **A:** Simulated Annealing at $\alpha = 0.3$, **B:** EdMC at $\alpha = 0.3$ (bottom) and $\alpha = 0.6$ (top). See text for the details of the procedure. Notice the difference in the $y$ axes scales. For both methods, 100 samples were tested for each value of $N$. Color shades reflect data density. Empty circles and squares represent medians, error bars span the 5-th to 95-th percentile interval. The dashed lines are fitted curves: the SA points are fitted by an exponential curve $\exp(a + bN)$ with $a = 8.63 \pm 0.06$, $b = (8.79 \pm 0.08) \cdot 10^{-3}$; the EdMC points are fitted by two polynomial curves $aN^b$ with $a = 0.54 \pm 0.04$, $b = 1.23 \pm 0.01$ for $\alpha = 0.3$, and with $a = 0.14 \pm 0.02$, $b = 1.74 \pm 0.02$ for $\alpha = 0.6$.

tanh$^{-1}(p)$ with $p = 0.4$, and ran the Monte Carlo procedure directly at $y = \infty$; if a solution was not found, we increased $p$ by a step of 0.1 and continued from the last accepted configuration, up to $p = 0.9$ if needed. Since we worked at $y = \infty$, we only needed to test each spin flip at most once before abandoning the search and increasing $p$. This procedure allowed us to find a solution in all cases.

The results are shown in Fig. 5, in log-log scale. For SA (panel A in the figure), the behavior is clearly exponential at $\alpha = 0.3$, and missing altogether for $\alpha = 0.6$. For EdMC (panel B in the figure), the data is well fit by polynomial curves, giving a scaling $\sim N^{1.23}$ for $\alpha = 0.3$ and $\sim N^{1.74}$ for $\alpha = 0.6$. Also note the difference of several orders of magnitude in the ranges of the $y$ axes in the two panels.

From the theoretical analysis, and the results shown in Figs. 1 and 3, it could be expected that EdMC should be able to find a solution at least until $\alpha \sim 0.75$ when the entropy curves
lose their monotonicity, and therefore be on par with reinforced Belief Propagation [17] and reinforced Max-Sum [18] in terms of algorithmic capacity (though being much slower in terms of absolute solving times), if following a cooling procedure on $y$. Assessing this in detail however would require even more extensive testing and goes beyond the scope of the present work.

Finally, we also tested SA using a simple variant of the energy function, in which a rectified linear function $f(x) = \max(0, x)$ is used instead of the step function $\Theta(x)$ in eq. (8), and verified that, while the performance indeed improves, the qualitative picture remains unchanged.

**B. Extensions: the K-SAT case and heuristic improvements**

The results we have displayed for the Binary Perceptron rely on a general scheme that in principle can be applied to other CSPs (or optimization problems). The main bottleneck in implementing such extensions resides in the possibility of computing the local entropy efficiently, e.g. by BP or some other sampling technique. As proof of concept we apply EdMC to the very well studied case of random $K$-SAT [3, 19, 20] focusing on the non trivial case $K = 4$, at various $N$ and $\alpha$. Random 4-SAT is characterized by three different regimes[21, 22]: For $\alpha < \alpha_d = 9.38$ the phase is RS and the solution space is dominated by a connected cluster of solutions with vanishing correlations among far apart variables. For $\alpha_d < \alpha < \alpha_c = 9.547$ the dominant part of the solution space brakes into an exponential number of clusters that have an extensive internal entropy. Long range correlations do not vanish. For $\alpha_c < \alpha < \alpha_s = 9.931$ the solution space is dominated by a sub-exponential number of clusters. Eventually for $\alpha > \alpha_s$ the problem becomes unsatisfiable. The hard region for random 4-SAT is $\alpha \in [\alpha_d, \alpha_s]$, i.e. where long range correlations do not vanish. In such region SA are expected to get stuck in glassy states and most of the heuristics are known to fail.

In the RS regime, EdMC succeeds in finding a solution in a small number of steps, confirming the smooth nature of the objective function. Typical trajectories for different values of $N$ are depicted in Figure 6A. Figure 6B shows the scaling behavior with $N$, which is polynomial ($\sim N^{1.15}$) as in the case of the Perceptron.

In the hard phase the method suffers from the lack of convergence of BP. Even if BP
Figure 6. Random 4-SAT, $\alpha = 8.0$ (easy phase), EdMC results with $y = \infty$ and $\gamma = \tanh^{-1}(0.3)$. 

A. Typical trajectories at different values of $N$, from 500 to 10000 (bottom to top), in log-log scale. B. Number of iterations to reach 0 energy, in log-log scale, as a function of the problem size $N$. Color shades reflect data density. Empty circles represent medians, error bars span the 5-th to 95-th percentile interval. The data is well fitted by a polynomial curve $aN^b$ (blue line), with $a = 1.94 \pm 0.15$, $b = 1.15 \pm 0.01$.

(technically the 1-RSB solution with $m = 1$) would converge up to the condensation point $\alpha_c$, the addition of the external fields prevent BP from converging even below such point. These are expected results that could be solved by resorting to a 1-RSB cavity algorithm to compute the local entropy. While certainly interesting, this is beyond the scope of this paper. For the sake of simplicity we decided to adopt simple heuristic solutions just to show that the overall method is effective.

In cases in which BP does not converge, we take as a proxy for $F$ its average $\bar{F}$ over a sufficient number of BP iterations. While this trick typically leads to a solution of the problem, it has the drawback of making the overall Monte Carlo procedure slow. To overcome this difficulty, we simply improve the choice of the flipping step by using the information contained in the cavity marginals in order to effectively guide the system into a state of high local density of solutions. The heuristic turns out to be much faster and capable of solving hard instances up to values of $\alpha$ close to the SAT/UNSAT threshold (see Fig. 7). The same heuristic has also been tested in the Perceptron learning problem with excellent results at high values of $\alpha$. 
The main step of the heuristic method consists in performing an extensive number of flipping steps at each iteration in the direction of maximum free energy, choosing the variables to flip from the set of \( x_i \)'s whose cavity marginals in absence of the external field \( h_i \) are not in agreement with the direction \( \tilde{x}_i \) of the field itself (see Appendix A for a precise definition of the marginals \( h_i \)). Let us call \( V \) the set of such variables, in a ranked order with respect to the difference between the external and the cavity fields, such that the ones with the largest difference come first. In the spirit of MCMCs, we propose a collective flip of all the \( V \) variables and compute the new value of \( F \). The collective flip is always accepted if there is an increase in free energy, otherwise it is accepted with probability \( e^{y \Delta F} \), where \( \Delta F \) is the free energy difference. When a collective flip is accepted, a new set \( V \) is computed. If, on the contrary, the flips are rejected, a new collective flip is proposed, simply eliminating the last variable in the ranked set \( V \), and the procedure is repeated until the set is empty. In the general case this procedure quickly leads to a solution with zero energy. If all the collective flips in \( V \) are rejected, the procedure is terminated, and a standard EdMC is started from the last accepted values of \( \tilde{x}_i \).

As it turns out, most of these collective moves are accepted immediately. The interpretation is that these moves try to maximize, at each step, the local contributions \( F_i \)'s associated to each variable \( x_i \) in the Bethe free energy, in presence of an external field \( \gamma \tilde{x}_i \).

As for standard EdMC, we can additionally employ an annealing strategy, by which \( y \) is progressively increased during the iteration, and a ‘scoping’ strategy, i.e. a gradual increase of the external field \( \gamma \) as well. The resulting algorithm is detailed in Algorithm 1.

Of the two strategies, annealing and scoping, the latter seems to be far more important in practice, and in many cases crucial to produce a quick solution: as \( \gamma \) is increased, smaller regions are progressively observed, and this focus can eventually lead the search into a given compact cluster of solutions, a region sufficiently dense so that Replica Symmetry locally holds. Indeed, in the typical observed trajectory of this algorithm in the presence of the scoping dynamics, even when BP suffers from convergence issues in the first steps, convergence is restored when the external fields vector \( \tilde{x} \) gets close to a region of high solution density. Both strategies, scoping and annealing, have been used to maximize the probability of success of the algorithm in the hard phase of the \( K \)-SAT problem in the simulations showed in Fig. 7.
Algorithm 1: Heuristic EdMC with Annealing and Scoping.

**Input:** problem sample; parameters $t_{\text{max}}$, $t_{\text{step}}$, $y$, $\gamma$, $f_y$ and $f_\gamma$

1. Randomly initialize $\tilde{x}_0^0$. Alternatively, run BP with $\gamma = 0$ and set $\tilde{x}_0^0 = \text{sign}(h_i)$
2. Run BP with external fields $\gamma \tilde{x}_0^0$
3. Compute free energy $F^0$ from BP fixed point ($\bar{F}^0$ if BP does not converge)
4. $t \leftarrow 0$
5. **while** $t \leq t_{\text{max}}$ **do**
6. Retrieve fields $h_i^t$ ($\bar{h}_i^t$ if BP did not converge)
7. **for** $i = 1$ to $N$ **do**
8. $\Delta_i \leftarrow \tilde{x}_i^t (\gamma \tilde{x}_i^t - h_i^t)$ Collect $V = \{i \mid \Delta_i > 0\}$ and sort it in descending order of $\Delta_i$
9. $\text{accepted} \leftarrow \text{FALSE}$
10. **while** NOT $\text{accepted}$ **do**
11. Propose a flip of the $\tilde{x}_i^t$ for all $i \in V$, producing $\tilde{x}^{t+1}$
12. Run BP with new proposed external fields $\gamma \tilde{x}_i^{t+1}$
13. Compute free energy $F^{t+1}$ from BP fixed point ($\bar{F}^{t+1}$ if BP does not converge)
14. **with probability** $e^{y(F^{t+1} - F^t)}$ **do** $\text{accepted} \leftarrow \text{TRUE}$
15. **if** NOT $\text{accepted}$ **then**
16. Remove the last element from $V$
17. **if** $|V| = 0$ **then** **exit** and run EdMC with $\tilde{x}^t$ as initial configuration
18. **end**
19. $t \leftarrow t + 1$
20. Compute energy $E$ of configuration $\tilde{x}^t$
21. **if** $E = 0$ **then** retrieve solution $\tilde{x}^* = \tilde{x}^t$ and **exit** **if** $t \equiv 0$ (mod $t_{\text{step}}$) **then**
22. **Annealing:** $y \leftarrow y \times f_y$
23. **Scoping:** $\gamma \leftarrow \gamma \times f_\gamma$ (run BP and update $F^t$)
24. **end**
25. **end**
We recently demonstrated the relevance of a probability measure based on the local entropy in the theoretical analysis of sub-dominant clusters in Constraint Satisfaction Problems [7]. In the present work, we extended on the previous analysis and introduced EdMC, a novel method for efficiently sampling over solutions in single instances of CSPs.

At variance with standard Monte Carlo methods, we never make use directly of the energy information: minimization of energy naturally emerges from the maximization of local entropy. What we propose here is thus a radically different perspective for optimization problems, based on the possibility of estimating the local entropy, a quantity that can effectively guide an MCMC straight into a region with a high density of solutions, thus providing a solver. The effectiveness of our Entropy-driven Monte Carlo may be understood...
in terms of a high level of smoothing in the local entropy landscape. This is evident if we compare a zero temperature EdMC to an energy guided SA with low cooling rate: the former is orders of magnitude faster in terms of attempted moves, and does not suffer from trapping in local minima. The procedure can even be made largely more efficient by a very simple heuristic.

In order to estimate the local entropy, we rely on BP, which itself can often be heuristically modified to become a solver (e.g. by introducing decimation or reinforcement schemes). However, those heuristics are not under control, while the scheme we propose here has a clear theoretical interpretation. BP is constructed on a cavity approximation scheme that strongly depends on the local factorization properties of the CSPs as well as on the global phase space structure, which is in general dependent on the number of constraints. The validity of cavity approximation has to be assessed for each problem at hand. It is very intriguing to think of simpler estimations for local entropy that could not rely on the convergence of BP equations. On the one hand, we have shown that even when convergence is not guaranteed at all, a simple averaging of messages could give useful information and lead to a solution in a small number of steps, implying that even an imprecise estimate of the local entropy is sufficient in these cases. Besides, the kinetic accessibility of sub-domiant clusters by simple learning protocols suggests that one could consider the general problem of engineering simple dynamical processes governed by the measure that we introduced in Eqs. (3-5). This subject is currently under investigation.

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Appendix A: Belief Propagation

In this section, we briefly introduce the Belief Propagation (BP) algorithm in general, define the quantities used by EdMC, and explicitly write the relevant expressions for the cases of the Binary Perceptron and the $K$-SAT problems. We will make use of the notation introduced in Sec. 1A.
1. General BP scheme

One common method for representing an instance of a CSP is to draw a bipartite Factor Graph, where each factor node stands for a constraint $\psi_{\mu}$, each variable node stands for a variable $x_i$, and each edge connects a factor node $\mu$ with a variable node $i$ if $i \in \partial \mu$, or equivalently $\mu \in \partial i$. This kind of graphical model representation is very helpful for understanding the basic dynamics of message passing methods such as BP.

Belief Propagation can be considered as a tool for an efficient marginalization of a complicated probability distribution that can be written as a product of local interaction terms. This is obviously the case of the Gibbs distribution associated to the Hamiltonian (1), which reads:

$$p_G(x) = \frac{1}{Z} \prod_{\mu} e^{-\beta E_{\mu}(x_{\partial \mu})}$$

In full generality, BP equations are a set of coupled nonlinear equations for the cavity messages $\{u_{i\rightarrow \mu}, \hat{u}_{\mu \rightarrow i}\}$, which can be viewed as messages associated to each link in the Factor Graph. For a Hamiltonian of the form (1), the BP equations are the following:

$$u_{i\rightarrow \mu}(x_i) \propto \prod_{\nu \in \partial i \setminus \mu} \hat{u}_{\nu \rightarrow i}(x_i) \quad (A1)$$

$$\hat{u}_{\mu \rightarrow i}(x_i) \propto \sum_{\{x_j\}_{j \neq i}} e^{-\beta E_{\mu}(x_{\partial \mu})} \prod_{j \in \partial \mu \setminus i} u_{j\rightarrow \mu}(x_j) \quad (A2)$$

A common way of solving these equations is by iteration, until convergence to a fixed point $\{u^*_{i\rightarrow \mu}, \hat{u}^*_{\mu \rightarrow i}\}$ is established. Fixed point messages may then be used to compute local joint marginals and other interesting macroscopic quantities such as the average energy and the free energy of the system. As explained in Sec. II B, one can also extract useful information from cavity messages themselves, and rely on them to construct a very efficient optimization procedure for the free energy. Of course, approximations for the true marginals and free energy can be obtained by means of instantaneous values $\{u^t_{i\rightarrow \mu}, \hat{u}^t_{\mu \rightarrow i}\}$ at a given computing time $t$, or by averaging them over the course of the BP iterations: we exploit this fact when dealing with regimes where the convergence of BP is hard if not impossible (see Sec. II B).

Non-cavity marginals over variables can be computed at the fixed point as:

$$u_i(x_i) \propto \prod_{\nu \in \partial i} \hat{u}_{\nu \rightarrow i}(x_i) \quad (A3)$$
The modified system obtained by adding the interaction term \( \gamma \tilde{x} \cdot x \) of eq. (5) introduces additional terms to eqs. (A1) and (A3):

\[
u_{i \to \mu} (x_i; \tilde{x}_i) \propto e^\gamma \tilde{x}_i x_i \prod_{\nu \in \partial \mu \setminus \mu} \hat{u}_{\nu \to \mu} (x_i)
\]

\[
u_i (x_i; \tilde{x}_i) \propto e^\gamma \tilde{x}_i x_i \prod_{\nu \in \partial \mu} \hat{u}_{\nu \to \mu} (x_i)
\]

In the heuristic version of EdMC presented in Sec. II B (Algorithm 1), we consider the case of binary spins \( x_i = \pm 1 \) and we use the cavity magnetization fields in absence of the external fields. These are defined from expression (A3) as:

\[
h_i = \tanh^{-1} (u_i (1) - u_i (-1))
\]

The local free entropy \( F (\tilde{x}, \gamma) \) of eq. (3) can be computed from the fixed point messages in the zero-temperature limit \( \beta \to \infty \) in terms of purely local contributions from variables, edges and factor nodes:

\[
F (\tilde{x}, \gamma) = \frac{1}{N} \sum_{\mu} \left( F_{\mu} (\tilde{x}, \gamma) + \sum_{i \in \partial \mu} F_{i \to \mu} (\tilde{x}, \gamma) \right) - \frac{1}{N} \sum_{i} (|\partial i| - 1) F_{i} (\tilde{x}, \gamma)
\]

where:

\[
F_{\mu} (\tilde{x}, \gamma) = \log \left( \sum_{\{x_{\partial \mu} : E(x_{\partial \mu}) = 0\}} \prod_{i \in \partial \mu} \nu_{i \to \mu} (x_i; \tilde{x}_i) \right)
\]

\[
F_{i \to \mu} (\tilde{x}, \gamma) = \log \left( \sum_{x_i} e^{\gamma \tilde{x}_i x_i} \prod_{\nu \in \partial \mu \setminus \mu} \hat{u}_{\nu \to \mu} (x_i) \right)
\]

\[
F_{i} (\tilde{x}, \gamma) = \log \left( \sum_{x_i} e^{\gamma \tilde{x}_i x_i} \prod_{\mu \in \partial \mu} \hat{u}_{\mu \to \mu} (x_i) \right)
\]

The overlap \( S (\tilde{x}, \gamma) = \frac{1}{N} \langle \tilde{x} \cdot x \rangle \) and the local entropy \( \mathcal{J} (\tilde{x}, \gamma) \) can be computed as:

\[
S (\tilde{x}, \gamma) = \frac{1}{N} \sum_{i} \tilde{x}_i \sum_{x_i} x_i u_i (x_i; \tilde{x}_i)
\]

\[
\mathcal{J} (\tilde{x}, \gamma) = F (\tilde{x}, \gamma) - \gamma S (\tilde{x}, \gamma)
\]

These expressions are used in Sec. 3, where \( F (\tilde{x}, \gamma) \) is optimized over \( \tilde{x} \) and they are averaged over many realizations of the patterns to compare them to the theoretical expression of eq. (6).
2. BP for the binary perceptron

The BP equations for a given instance \((\xi^\mu, \sigma^\mu)\), \(\mu = 1...\alpha N\) are most easily written in terms of cavity magnetizations \(m_{i\rightarrow\mu} \propto u_{i\rightarrow\mu} (+1) - u_{i\rightarrow\mu} (-1)\) and \(\hat{m}_{\mu \rightarrow i} \propto \hat{u}_{\mu \rightarrow i} (+1) - \hat{u}_{\mu \rightarrow i} (-1)\). Note that it is always possible to set \(\forall \mu: \sigma^\mu = 1\) without loss of generality, by means of the simple gauge transformation \(\xi^\mu_i \rightarrow \sigma^\mu \xi^\mu_i\). With these simplification, equations (A1, A2) become:

\[
m_{i\rightarrow\mu} = \tanh \left( \sum_{\nu \neq \mu} \tanh^{-1} (\hat{m}_{\nu \rightarrow i}) \right) \tag{A13}
\]

\[
\hat{m}_{\mu \rightarrow i} = \frac{\sum_{s=-\xi_i}^{N-1} D_{\mu \rightarrow i} (s) - \sum_{s=\xi_i}^{N-1} D_{\mu \rightarrow i} (s)}{\sum_{s=-\xi_i}^{N-1} D_{\mu \rightarrow i} (s) + \sum_{s=\xi_i}^{N-1} D_{\mu \rightarrow i} (s)} \tag{A14}
\]

where

\[
D_{\mu \rightarrow i} (s) = \sum_{\{x_j\}_{j \neq i}} \delta \left( s, \sum_j x_j \xi_j \right) \prod_{j \neq i} \frac{1 + x_j m_{j \rightarrow \mu}}{2} \tag{A15}
\]

is the convolution of the all cavity messages \(m_{j \rightarrow \mu}\) impinging on the pattern node \(\mu\), except for \(m_{i \rightarrow \mu}\): it is thus the (cavity) distribution of the total synaptic input for pattern \(\mu\), in absence of the synapse \(i\). The complexity of the second update is at most \(O(N^2)\) with an appropriate pre-computation of cavity convolutions. When one deals with the case of \(N \gg 1\) and an extensive number of patterns, a common and simple strategy is to adopt a Gaussian approximation \(\hat{D}_{\mu \rightarrow i} (s) = \frac{1}{b_{\mu \rightarrow i}} G \left( \frac{s-a_{\mu \rightarrow i}}{b_{\mu \rightarrow i}} \right)\) for the distribution \(D_{\mu \rightarrow i} (s)\), where \(G(s)\) denotes the normal distribution. It suffices then to compute the mean \(a_{\mu \rightarrow i}\) and variance \(b_{\mu \rightarrow i}^2\) of the distribution \(\hat{D}_{\mu \rightarrow i} (s)\), whose dependence on cavity messages \(m_{j \rightarrow \mu}\) is easily determined from the central limit theorem:

\[
a_{\mu \rightarrow i} = \sum_{j \neq i} \xi_j^\mu m_{j \rightarrow \mu} \tag{A16}
\]

\[
b_{\mu \rightarrow i}^2 = \sum_{j \neq i} (1 - m_{j \rightarrow \mu}^2) \tag{A17}
\]

(analogous non-cavity quantities \(a_{\mu}\) and \(b_{\mu}\) are computed by summing over all indices \(j\)). By doing so, equation (A14) becomes:

\[
\hat{m}_{\mu \rightarrow i} = \xi_i g (a_{\mu \rightarrow i}, b_{\mu \rightarrow i}) \tag{A18}
\]
where
\[ g(a, b) = \frac{H(a - 1) - H(a + 1)}{H(a - 1) + H(a + 1)} \]
and we used the function \( H(x) = \frac{1}{2} \text{erfc} \left( \frac{x}{\sqrt{2}} \right) \).

The free-entropy \( F_{\text{perc}} \) can be easily obtained by eq. (A7) putting \( \gamma = 0 \). In our Gaussian approximation, the expression can be written as:
\[ F_{\text{perc}} = \frac{1}{N} \sum_{\mu} \log \left( H \left( \frac{a_{\mu}}{b_{\mu}} \right) \right) - \frac{1}{N} \sum_{i, \mu} \log \left( 1 + m_{i \rightarrow \mu} \hat{m}_{\mu \rightarrow i} \right) + \frac{1}{N} \sum_{\mu} \log \left[ \prod_{\mu} (1 + \hat{m}_{\mu \rightarrow i}) + \prod_{\mu} (1 - \hat{m}_{\mu \rightarrow i}) \right] \]

The total number of solutions for a given instance can be determined by means of the entropy:
\[ S_{\text{perc}} = \frac{1}{N} \sum_{\mu} \log \left( H \left( \frac{a_{\mu}}{b_{\mu}} \right) \right) - \frac{1}{N} \sum_{i, \mu} \left[ \frac{1 + m_{i}}{2} \log \left( \frac{1 + m_{i \rightarrow \mu}}{2} \right) + \frac{1 - m_{i}}{2} \log \left( \frac{1 - m_{i \rightarrow \mu}}{2} \right) \right] + \frac{M - 1}{N} \sum_{i} \left[ \frac{1 + m_{i}}{2} \log \left( \frac{1 + m_{i}}{2} \right) + \frac{1 - m_{i}}{2} \log \left( \frac{1 - m_{i}}{2} \right) \right] \]

Consistently with the theoretical predictions, BP equations always converge for \( \alpha < \alpha_c \).

Indeed, Replica Symmetry holds with the identification of states as the dominant isolated configurations, this being evident in the proportionality relation between RS and RSB free-energy [11], with an intra-state overlap (RSB parameter) \( q_1 \) equal to 1. The entropy decreases monotonically with \( \alpha \) and, provided \( N \) is high enough, it vanishes at the critical threshold \( \alpha_c \sim 0.833 \) [11].

Very interestingly, if one slightly modifies the original equations with the introduction of a ‘reinforcement term’, much similar to a sort of smooth decimation procedure, BP becomes a very efficient solver that is able to find a solution with probability 1 up to \( \alpha \sim 0.74 \) [17]. Reinforced BP equations can be further simplified, this leading to a dramatic reduction in update complexity. The resulting on-line algorithms, SBPI [23] and CP+R [24] are able to achieve a slightly lower capacity (\( \alpha \sim 0.69 \)). As we pointed out in the Introduction, Sec. I, the performances of all the cited algorithms seem to be directly affected by large sub-dominant clusters: these high entropy states happen to be easily accessible, while the dominant isolated solutions are very hard (if not impossible) to find efficiently by simple learning methods.
Introducing the external fields $\gamma \bar{x}_i$ of eq. (4) is very simple (cf. eqs. (A4) and (A5)).

Eq. (A13) for the cavity magnetization is modified as:

$$m_{i \to \mu} = \tanh \left( \sum_{\nu \neq \mu} \tanh^{-1}(\hat{m}_{\nu \to i}) + \gamma \bar{x}_i \right)$$  \hspace{1cm} (A22)

and similarly for the total magnetization: $m_i = \tanh \left( \sum_{\mu} \tanh^{-1}(\hat{m}_{\mu \to i}) + \gamma \bar{x}_i \right)$. The local free entropy is also simply given by the expression $F_{\text{perc}}(\bar{x}, \gamma) = F_{\text{perc}}(\bar{x}, \gamma) + \gamma S(\bar{x}, \gamma)$ using eqs. (A21) and (A11) with the modified magnetizations. The cavity magnetization fields in absence of the external fields, eq. (A6), are:

$$h_i = \sum_{\mu} \tanh^{-1}(\hat{m}_{\mu \to i})$$  \hspace{1cm} (A23)

3. BP for K-SAT

The Belief Propagation equations for the K-SAT problem are most easily written with a parametrization of the BP messages $\{u_{i \to \mu}, \hat{u}_{\mu \to i}\}$ in terms of the quantities $\{\zeta_{i \to \mu}, \eta_{\mu \to i}\}$, where $\zeta_{i \to \mu}$ is the probability that $x_i$ does not satisfy clause $\mu$ in absence of this clause, and $\eta_{\mu \to i}$ is the probability that all the variables in clause $\mu$ except $i$ violate the clause. With this choice, and calling $V(\mu)$ the set of variables in the constraint $\mu$, equation (A2) simply becomes:

$$\eta_{\mu \to i} = \prod_{j \in V(\mu) \setminus i} \zeta_{j \to \mu}$$  \hspace{1cm} (A24)

Equation (A1) for the variable node update is slightly more involved:

$$\zeta_{i \to \mu} = \frac{\prod_{\nu \in V_{\mu}^+(i)} (1 - \eta_{\nu \to i})}{\prod_{\nu \in V_{\mu}^-(i)} (1 - \eta_{\nu \to i}) + \prod_{\nu \in V_{\mu}^+(i)} (1 - \eta_{\nu \to i})}$$  \hspace{1cm} (A25)

where $V_{\mu}^+(i)$ (resp. $V_{\mu}^-(i)$) is the set of clauses $\nu$ in which variable $i$ is involved with a coupling $J_{i \nu}^\mu \neq J_{i \nu}^\nu$ (resp. $J_{i \nu}^\nu = J_{i \nu}^\mu$).

As for the perceptron, the free-entropy is obtained from expression (A7) at $\gamma = 0$:

$$F_{\text{SAT}} = \frac{1}{N} \sum_{\mu} \log \left( 1 - \prod_{i \in V(\mu)} \zeta_{i \to \mu} \right) - \frac{1}{N} \sum_{i} \sum_{\mu \in \partial i} \log \left( 1 - \zeta_{i \to \mu}^{-2} \right) +$$

$$+ \frac{1}{N} \sum_{i} \log \left[ \prod_{\nu \in V^+(i)} (1 - \eta_{\nu \to i}) + \prod_{\nu \in V^-(i)} (1 - \eta_{\nu \to i}) \right]$$  \hspace{1cm} (A26)
where $V^+(i)$ (resp. $V^-(i)$) is the set of all clauses $\mu$ in which variable $i$ is involved with $J_\mu^i = -1$ (resp. $J_\mu^i = 1$). Analogously, the entropy is obtained from the following expression, which only depends upon the messages $\eta_{\nu \to i}$:

$$S_{\text{SAT}} = \frac{1}{N} \sum_\mu \log \left[ \prod_{i \in V(\mu)} \left( \prod_{\nu \in V^+(i)} (1 - \eta_{\nu \to i}) + \prod_{\nu \in V^-(i)} (1 - \eta_{\nu \to i}) \right) - \prod_{i \in V(\mu)} \left( \prod_{\nu \in V^+(i)} (1 - \eta_{\nu \to i}) \right) \right]$$

$$+ \frac{1}{N} \sum_i (1 - |\partial i|) \log \left[ \prod_{\nu \in V^+(i)} (1 - \eta_{\nu \to i}) + \prod_{\nu \in V^-(i)} (1 - \eta_{\nu \to i}) \right]$$  \quad \text{(A27)}$$

In the chosen parametrization, the external fields $\gamma \tilde{x}_i$ may be easily introduced by means of $N$ additional single-variable ‘soft clauses’ $\tilde{C}_i$, which send fixed cavity messages to their respective variables, taking the value:

$$\eta_{\tilde{C}_i \to i} = \frac{2 \tanh \gamma}{1 + \tanh \gamma}$$  \quad \text{(A28)}$$

with the restriction that $\tilde{C}_i \in V^+(i)$ (resp. $\tilde{C}_i \in V^-(i)$) if $\tilde{x}_i = +1$ (resp. $\tilde{x}_i = -1$).

If we call $\tilde{V}^+(i)$, $\tilde{V}^-(i)$ the new set of clauses, enlarged so as to contain the $\tilde{C}_i$, the total magnetization is given by:

$$m_i = \frac{\prod_{\nu \in V^-(i)} (1 - \eta_{\nu \to i}) - \prod_{\nu \in V^+(i)} (1 - \eta_{\nu \to i})}{\prod_{\nu \in V^-(i)} (1 - \eta_{\nu \to i}) + \prod_{\nu \in V^+(i)} (1 - \eta_{\nu \to i})}$$  \quad \text{(A29)}$$

The cavity magnetization fields in absence of the external fields, eq. (A6), are simply given by:

$$h_i = \tanh^{-1} (m_i) - \gamma \tilde{x}_i$$  \quad \text{(A30)}$$

Convergence properties of equations (A24,A25) on single instances are deeply related to the Replica Symmetry Breaking scenario briefly discussed in the preceding section. The onset of long range correlations in clustered RSB phase prevents BP from converging.

While RSB limits the usefulness of BP (as well as reinforced BP) at high $\alpha$, ideas from the 1-RSB cavity method, when applied to the single case without the averaging process, have led to the introduction of a powerful heuristic algorithm, Survey Propagation (SP) [3, 25], which is able to solve $K$-SAT instances in the hard phase, almost up to the UNSAT threshold.
Appendix B: Details of the large deviations analysis for the binary Perceptron

Learning problem

In this section, we provide all technical details of the analysis of the reweighted free energy function of eq. (5) of Sec. I A for the case of the Perceptron Learning problem with binary synapses of Sec. I A 2 a. The results of this analysis are presented in Sec. II A 1.

However, the notation in this section will differ at times from the one in the main text, to make it more similar to the one used in [7], and so that this section is mostly self-contained.

1. Setting the problem and the notation

We generate patterns by drawing the inputs as random i.i.d. variables \( \xi_i \in \{-1, +1\} \) with distribution \( P(\xi_i) = \frac{1}{2} \delta (\xi_i - 1) + \frac{1}{2} \delta (\xi_i + 1) \). Without loss of generality, we assume that the desired output of all patterns is 1.

We consider the learning problem of correctly classifying a set of \( \alpha N \) patterns \( \{\xi^\mu\} \) (where \( \mu = 1, \ldots, \alpha N \)). We define, for any vector of synaptic weights \( W = \{W_i\}_{i=1,\ldots,N} \) with \( W_i \in \{-1, +1\} \) the quantity

\[
X_{\xi}(W) = \prod_{\mu} \Theta \left( \frac{1}{\sqrt{N}} \sum_i W_i \xi^\mu_i \right)
\]

(B1)

such that the solutions of the learning problem are described by \( X_{\xi}(W) = 1 \). The factor \( 1/\sqrt{N} \) has been added to account for the scaling of the effective fields.

Note that throughout this section we will use the index \( i \) for the synapses and \( \mu \) for the patterns. In all sums and products, the summation ranges are assumed implicitly, e.g. \( \sum_i \equiv \sum_{i=1}^N \). Also, all integrals are assumed to be taken over \( \mathbb{R} \) unless otherwise specified. The letters \( a, b, c \) and \( d \) will be reserved for replica indices (see below). Finally, when we will make the 1-RSB Ansatz, we will also use \( \alpha, \beta, \alpha' \) and \( \beta' \) for the replica indices; it should be clear from the context that these do not refer to the capacity \( \alpha \) or the inverse temperature \( \beta \) in those cases.

We write the number of solutions as:

\[
N_{\xi} = \sum_{\{W\}} X_{\xi}(W)
\]

(B2)
We want to study the solution space of the problem in the following setting: we consider a set of reference configurations, each of which has an associated set of solutions that are constrained to have a certain overlap $S$ with it.

In the following, we indicate with $\tilde{W}$ the reference configurations, and with $W$ the other solutions. In general we use a tilde for all the quantities that refer to the reference configurations.

Let us define then:

$$N_{\xi}(\tilde{W}, S) = \sum_{\{\tilde{W}\}} X_{\xi}(W) \delta \left( \sum_{i} W_i \tilde{W}_i - SN \right)$$

(B3)

(where $\delta$ is the Dirac-delta distribution[26]), i.e. the number of solutions $W$ that have overlap $S$ with (or equivalently, distance $1 - \frac{S}{2}$ from) a reference configuration $\tilde{W}$. We then introduce the following quenched free energy:

$$F(S, y) = -\frac{1}{Ny} \langle \log (\Omega(S, y)) \rangle_{\{\xi\}} = -\frac{1}{Ny} \left\langle \log \left( \sum_{\{\tilde{W}\}} N_{\xi}(\tilde{W}, S)^y \right) \right\rangle_{\{\xi\}}$$

(B4)

where $\Omega(S, y)$ is the partition function and $y$ has the role of an inverse temperature. This is the free energy density of a system where the configuration is described by $\tilde{W}$ and the energy is given by minus the entropy of the other solutions with overlap $S$ from it.

This expression is almost equivalent to eq. 5 in the main text, except that we used the overlap $S$ as a control parameter instead of the coupling $\gamma$, by using a hard constraint (the delta distribution in eq. B3) rather than a soft constraint (the exponential in eq. 4). The two parameters are conjugates. The main advantage of using $\gamma$ is that it is easier to implement using the BP algorithm, which is why we used it for the EdMC algorithm. The advantage of using $S$ is that it provides a more general description: while in large portions of the phase space the relationship between $\gamma$ and $S$ is bijective (and thus the two systems are equivalent), some regions of the phase space at large $\alpha$ can only be fully explored with by constraining $S$, and thus we have used this system for the theoretical analysis.

The main goal is that of studying the ground states of the system, i.e. taking the limit of $y \to \infty$. This limit allows us to seek the reference configuration $\tilde{W}$ for which the number of solutions at overlap $S$ with it is maximal, and to derive an expression for the entropy $\mathcal{S}(S, y) = \langle \log N_{\xi}(\tilde{W}, S) \rangle$ of the surrounding solutions, which we call local entropy. As
we shall see, we find that $\mathcal{S}(S, \infty)$ is always positive for $\alpha < \alpha_c$ when $S \to 1$, indicating the presence of dense clusters of solutions.

In the remainder, we will generally use the customary notation $\int d\mu(W)$ or $\prod_i d\mu(W_i)$ (in stead of $\sum_W$ or $\sum\{W\}$) to denote the integral over possible values of the weights; since we assume binary weights, we will have:

$$d\mu(W) = (\delta(W - 1) + \delta(W + 1)) dW$$

2. Entropy and Complexity

a. Replica trick

In order to compute the quantity of eq. (B4), we use the replica trick. We will use $n$ to denote the number of replicas of the reference configurations, and the letters $c$ and $d$, with $c, d \in \{1, \ldots, n\}$, as their replica indices.

We will also write $\mathcal{N}\left(\tilde{W}, S\right)^y$ as a product of $y$ “local” replicas. Note that we will have a different set of local replicas for each replicated reference configuration, so that the local replicas are $yn$ in total. We use the indices $a$ and $b$ to denote these local replicas (each of which will also have a reference replica index $c$), i.e. $a, b \in \{1, \ldots, y\}$.

Therefore, we need to compute:

$$\lim_{n \to 0} \left\langle \Omega(S, y)^n \right\rangle_{\{\xi^\mu\}} = (B5)$$

As a first step, we substitute the arguments of the theta functions in the $\Theta$ terms via Dirac-delta functions:

$$\prod_{ca\mu} \Theta\left(\frac{1}{\sqrt{N}} \sum_i W_i^{ca} \xi_i^\mu\right) = \prod_{ca\mu} d\lambda^{ca}_{\mu} \delta\left(\lambda^{ca}_{\mu} - \frac{1}{\sqrt{N}} \sum_i W_i^{ca} \xi_i^\mu\right) \prod_{ca\mu} \Theta\left(\lambda^{ca}_{\mu}\right) \quad (B6)$$

Then, we expand the delta functions using their integral representation:

$$\delta\left(\lambda^{ca}_{\mu} - \frac{1}{\sqrt{N}} \sum_i W_i^{ca} \xi_i^\mu\right) = \int d\tilde{\lambda}^{ca}_{\mu} \exp\left(i \tilde{\lambda}^{ca}_{\mu} \lambda^{ca}_{\mu} - i \tilde{\lambda}^{ca}_{\mu} \frac{1}{\sqrt{N}} \sum_i W_i^{ca} \xi_i^\mu\right) \quad (B7)$$

With these, we can factorize the expression where the patterns are involved, so we can compute the averages over the patterns independently for each $\mu$ and for each $i$, and expand...
for large $N$:

$$\prod_i \int (\xi_i^\mu \, d\xi_i^\mu) \exp \left( -\frac{i}{\sqrt{N}} \xi_i^\mu \left( \sum_{ca} W_{c}^{ca} \hat{\lambda}_{ca}^\mu \right) \right) =$$

$$\simeq \exp \left( -\frac{1}{2N} \sum_i \left( \sum_{ca} W_{c}^{ca} \hat{\lambda}_{ca}^\mu \right)^2 \right)$$

$$= \exp \left( -\frac{1}{2} \left( \sum_{cadb} \hat{\lambda}_{ca}^\mu \hat{\lambda}_{db}^\mu \left( \frac{1}{N} \sum_i W_{c}^{ca} W_{i}^{db} \right) \right) \right) \quad (B8)$$

Next, we introduce order parameters for the overlaps via delta functions (we already have the one for the overlaps $\frac{1}{N} \sum W_{c}^{ca} \hat{W}_{i}^{c}$ which must be equal to $S$), and use the expressions (B6), (B7) and (B8) in eq. (B5), to get:

$$\langle \Omega (S, y)^n \{\xi^\mu\} \rangle = \int \prod_{ic} d\mu \left( \hat{W}_{i}^{c} \right) \int \prod_{ia} d\mu \left( W_{i}^{ca} \right) \int \prod_{ca} \frac{d\hat{\lambda}_{ca}^\mu \, d\lambda_{ca}^\mu}{2\pi} \prod_\mu e^{i \left( \sum_{ca} \lambda_{ca}^\mu \hat{\lambda}_{ca}^\mu \right)} \times$$

$$\times \int \prod_{c,a>b} (dq_{ca,cb}^{ca,db} N) \delta \left( N q_{ca,cb}^{ca,db} - \sum_i W_{c}^{ca} W_{i}^{cb} \right) \times$$

$$\times \int \prod_{c>d,ab} (dq_{ca,db}^{ca,db} N) \delta \left( N q_{ca,db}^{ca,db} - \sum_i W_{c}^{ca} W_{i}^{db} \right) \times$$

$$\times \prod_{ca} \delta \left( NS - \sum_i W_{i}^{ca} \hat{W}_{i}^{c} \right) \prod_{ca} \Theta (\lambda_{ca}^\mu) \prod_\mu \exp \left( -\frac{1}{2} \sum_{ca} \hat{\lambda}_{ca}^\mu \right) \times$$

$$\times \prod_\mu \exp \left( -\sum_{c} \sum_{a>b} \hat{\lambda}_{ca}^\mu \hat{\lambda}_{cb}^\mu q_{ca,cb}^{ca,db} - \sum_{c>d} \sum_{ab} \hat{\lambda}_{ca}^\mu \hat{\lambda}_{db}^\mu q_{ca,db}^{ca,db} \right) \quad (B9)$$

Then we expand the deltas in the usual way introducing conjugate parameters $\hat{q}_{ca,db}^{ca,db}$ and $\hat{S}_{ca}^{ca}$, and rearrange the integrals such that we can factorize over $\mu$ (and therefore drop the $\mu$ index entirely) and over $i$ (and drop that index as well). We obtain:

$$\langle \Omega (S, y)^n \{\xi^\mu\} \rangle = \int \prod_{c,a>b} \left( \frac{dq_{ca,cb}^{ca,db} N}{2\pi} \right) \int \prod_{c>d,ab} \left( \frac{dq_{ca,db}^{ca,db} N}{2\pi} \right) \int \prod_{ca} \left( \frac{d\hat{S}_{ca}^{ca} N}{2\pi} \right)$$

$$e^{-N \left( \sum_{c} \sum_{a>b} q_{ca,cb}^{ca,db} q_{ca,db}^{ca,db} + \sum_{c>d} q_{ca,db}^{ca,db} \sum_{ca} S_{ca}^{ca} \right) G_{S}^{N} G_{E}^{N}} \quad (B10)$$

where $G_{S}$ and $G_{E}$ are the entropic and the energetic terms, respectively:

$$G_{S} = \int \prod_{c} d\mu \left( \hat{W}_{c}^{c} \right) \int \prod_{ca} d\mu \left( W_{c}^{ca} \right) \exp \left( \sum_{c} \sum_{a>b} \hat{q}_{ca,cb}^{ca,db} W_{c}^{ca} W_{i}^{cb} + \right.$$  

$$+ \sum_{c>d} \sum_{ab} \hat{q}_{ca,db}^{ca,db} W_{c}^{ca} W_{i}^{db} + \sum_{ca} \hat{S}_{ca}^{ca} W_{c}^{ca} \hat{W}_{c}^{c} \right) \quad (B11)$$
\[ G_E = \int \prod_{c\alpha} d\lambda^{c\alpha} d\hat{\lambda}^{c\alpha} e^{i (\sum_{\alpha} \lambda^{c\alpha} \lambda^{c\alpha})} \prod_{c\alpha} \Theta (\lambda^{c\alpha}) \exp \left( -\frac{1}{2} \sum_{c\alpha} (\hat{\lambda}^{c\alpha})^2 + \right) \]
\[ \sum_c \sum_{a>b} \hat{\lambda}^{c\alpha \hat{\lambda}^{c\beta}} q^{c\alpha,c\beta} - \sum_c \sum_{d>ab} \hat{\lambda}^{c\alpha} \hat{\lambda}^{db} q^{c\alpha,db} \right) \]

\[ b. \ The \ external \ 1\text{-}RSB \ Ansatz \]

As explained in the main text, we will make a 1-RSB Ansatz for the planted configurations. More specifically, we will divide the \( n \) replicas in \( \frac{n}{m} \) groups of \( m \) replicas each, with \( m \) the Parisi 1-RSB parameter over which we will subsequently optimize. Let us then introduce the multi-index \( c = (\alpha, \beta) \), where \( \alpha \in \{1, ..., n/m\} \) labels a block of \( m \) replicas, and \( \beta \in \{1, ..., m\} \) is the index of replicas inside the block. This induces the following structure for the overlap matrix \( q^{\alpha\beta, \alpha'\beta', a} \equiv q^{\alpha\alpha', \beta\beta'} \):

\[ q^{\alpha\beta, \alpha'\beta', b} = \begin{cases} 
1 & \text{if } \alpha = \alpha', \beta = \beta', a = b \\
q_2 & \text{if } \alpha = \alpha', \beta = \beta', a \neq b \\
q_1 & \text{if } \alpha = \alpha', \beta \neq \beta' \\
q_0 & \text{if } \alpha \neq \alpha'
\end{cases} \]

(B13)

The structure of the conjugated parameters matrix \( \hat{q}^{ca,db} \) is analogous. We also assume \( \hat{S}^{ca} = \hat{S} \). Note that \( \hat{S} \), being the conjugate of \( S \), takes the role of the soft constraint parameter \( \gamma \) of eq. 4 that is used throughout the main text. In fact, as already noted, studying the soft-constrained system of eq. 5 gives exactly the same results with \( \hat{S} = \gamma \), provided one makes an equivalent symmetric Ansatz on the overlap \( S \) as it is done for \( \hat{S} \) here.

c. Entropic term

Let us consider the entropic term in the 1-RSB Ansatz:

\[ G_S = \int \prod_{\alpha\beta} d\mu \left( \hat{W}^{\alpha\beta} \right) \int \prod_{\alpha\beta,a} d\mu (W^{\alpha\beta,a}) \exp \left( -\frac{\hat{q}_2}{2} \hat{q}_2 \right) + \frac{1}{2} \sum_{\alpha\beta} \left( \sum_a W^{\alpha\beta,a} \right)^2 \times \]
\[ \times \exp \left( \frac{\hat{q}_1 - \hat{q}_0}{2} \sum_{\alpha\beta,a} \left( \sum_{\beta,a} W^{\alpha\beta,a} \right)^2 + \frac{\hat{q}_0}{2} \left( \sum_{\alpha\beta,a} W^{\alpha\beta,a} \right)^2 + \hat{S} \sum_{\alpha\beta,a} \hat{W}^{\alpha\beta} \right) \]
By means of a Hubbard-Stratonovich transformation

\[
\exp \left( \frac{b}{2} x^2 \right) = \int Dz \exp \left( x \sqrt{b} z \right)
\]
on the term quadratic term \( (\sum_{\alpha \beta, a} W^{\alpha\beta; a})^2 \), everything factorizes over the replica index \( \alpha \), thus obtaining:

\[
G_S = e^{-\frac{\hat{q}_2}{2} n y} \int Dz_0 \left\{ \int \prod_{\beta} d\mu (\hat{W}^{\beta}) \int \prod_{\beta, a} d\mu (W^{\beta, a}) \exp \left( \frac{(\hat{q}_2 - \hat{q}_1)}{2} \sum_{\beta} \left( \sum_{a} W^{\beta, a} \right)^2 \right) \times \exp \left( \frac{(\hat{q}_1 - \hat{q}_0)}{2} \left( \sum_{\beta, a} W^{\beta, a} \right)^2 + z_0 \sqrt{\hat{q}_0} \sum_{\beta, a} W^{\beta, a} + S \sum_{\beta, a} \hat{W}^{\beta} W^{\beta, a} \right) \right\}^{\frac{n}{m}} \quad (B15)
\]

Another transformation of the term \( (\sum_{\beta, a} W^{\alpha\beta, a}) \) allows to factorize over the index \( \beta \):

\[
G_S = e^{-\frac{\hat{q}_2}{2} n y} \int Dz_0 \left\{ \int Dz_1 \left\{ \int d\mu (\hat{W}) \int \prod_{a} d\mu (W^a) \exp \left( \frac{(\hat{q}_2 - \hat{q}_1)}{2} \left( \sum_{a} W^a \right)^2 \right) \times \exp \left( z_1 \sqrt{\hat{q}_1 - \hat{q}_0} \sum_{a} W^a + z_0 \sqrt{\hat{q}_0} \sum_{a} W^a + S \sum_{a} \hat{W} W^a \right) \right\}^{\frac{m}{m}} \right\}^{\frac{n}{m}} \quad (B16)
\]

and again on the term \( (\sum_{a} W^a)^2 \), with a final factorization over the index \( a \):

\[
G_S = e^{-\frac{\hat{q}_2}{2} n y} \int Dz_0 \left\{ \int Dz_1 \left\{ \int Dz_2 \int d\mu (\hat{W}) \left( \int d\mu (W) \exp \left( z_2 \sqrt{\hat{q}_2 - \hat{q}_1} W \right) \times \exp \left( z_1 \sqrt{\hat{q}_1 - \hat{q}_0} W + z_0 \sqrt{\hat{q}_0} W + S \hat{W} W \right) \right) \right\}^{\frac{m}{m}} \right\}^{\frac{n}{m}} \quad (B17)
\]

Let us then consider the specific case of binary variables \( W, \hat{W} \in \{-1, +1\} \) and perform the sum over \( W \) explicitly, thus obtaining:

\[
G_S = e^{-\frac{\hat{q}_2}{2} n y} \int Dz_0 \left\{ \int Dz_1 \left\{ \int Dz_2 \sum_{W=\pm 1} \left( \frac{2 \cosh \left( \hat{A} \left( z_0, z_1, z_2; \hat{W} \right) \right) \right) \right\}^{\frac{m}{m}} \right\}^{\frac{n}{m}} \quad (B18)
\]

where

\[
\hat{A} \left( z_0, z_1, z_2; \hat{W} \right) = z_2 \sqrt{\hat{q}_2 - \hat{q}_1} + z_1 \sqrt{\hat{q}_1 - \hat{q}_0} + z_0 \sqrt{\hat{q}_0} + S \hat{W} \quad (B19)
\]

Performing the limit \( n \to 0 \) we obtain:

\[
\log \frac{G_S}{n} = -\frac{\hat{q}_2}{2} y + G_S \quad (B20)
\]

where

\[
G_S = \frac{1}{m} \int Dz_0 \log \left( \int Dz_1 \left\{ \int Dz_2 \sum_{W=\pm 1} \left( \frac{2 \cosh \left( \hat{A} \left( z_0, z_1, z_2; \hat{W} \right) \right) \right) \right\}^{\frac{m}{m}} \right) \quad (B21)
\]
d. Energetic term

Let us plug the 1-RSB Ansatz (B13) in eq. (B12) and get:

\[
G_E = \prod_{\alpha, \beta, a} \frac{d\lambda^{\alpha,\beta,a} d\hat{\lambda}^{\alpha,\beta,a}}{2\pi} \prod_{\alpha, \beta, a} \Theta (\lambda^{\alpha,\beta,a}) \exp \left( i \sum_{\alpha, \beta, a} \lambda^{\alpha,\beta,a} \hat{\lambda}^{\alpha,\beta,a} - \frac{1}{2} \sum_{\alpha, \beta, a} (\hat{\lambda}^{\alpha,\beta,a})^2 \right) \times
\]

\[
\times \exp \left( -q_2 \sum_{\alpha, \beta} \sum_{a > b} \hat{\lambda}^{\alpha,\beta,a} \hat{\lambda}^{\alpha,\beta,b} - q_1 \sum_{\alpha, \beta > \beta'} \sum_{ab} \hat{\lambda}^{\alpha,\beta,a} \hat{\lambda}^{\alpha,\beta',b} \right) \times
\]

\[
\times \exp \left( -q_0 \sum_{a > a', \beta \beta'} \sum_{ab} \hat{\lambda}^{\alpha,\beta,a} \hat{\lambda}^{\alpha',\beta',b} \right)
\]

\[(B22)\]

We then use the formula

\[
\sum_{i>j} a_i a_j = \frac{1}{2} \left( \left( \sum_i a_i \right)^2 - \sum_i a_i^2 \right)
\]

for the various quadratic terms in \(\lambda\)'s and \(\hat{\lambda}\)'s in eq. (B22), thus obtaining:

\[
G_E = \prod_{\alpha, \beta, a} \frac{d\lambda^{\alpha,\beta,a} d\hat{\lambda}^{\alpha,\beta,a}}{2\pi} \prod_{\alpha, \beta, a} \Theta (\lambda^{\alpha,\beta,a}) \exp \left( i \sum_{\alpha, \beta, a} \lambda^{\alpha,\beta,a} \hat{\lambda}^{\alpha,\beta,a} - \frac{1}{2} \sum_{\alpha, \beta, a} (\hat{\lambda}^{\alpha,\beta,a})^2 \right) \times
\]

\[
\times \exp \left( -q_2 \sum_{\alpha, \beta} \left( \sum_a \hat{\lambda}^{\alpha,\beta,a} \right)^2 - \sum_a (\hat{\lambda}^{\alpha,\beta,a})^2 \right) \times
\]

\[
\times \exp \left( -q_1 \left( \sum_{\alpha, \beta', \beta} \left( \sum_a \hat{\lambda}^{\alpha,\beta,a} \right)^2 - \sum_{\beta, b} (\hat{\lambda}^{\alpha,\beta,a})^2 \right) \right) \times
\]

\[
\times \exp \left( -q_0 \left( \sum_{\alpha, \beta, a} \left( \sum_a \hat{\lambda}^{\alpha,\beta,a} \right)^2 - \sum_{\alpha, \beta} (\sum_a \hat{\lambda}^{\alpha,\beta,a})^2 \right) \right)
\]

\[(B23)\]

Let us then linearize the term multiplying \(q_0\) by means of a Hubbard-Stratonovich transformation, thereby factorizing over the replica index \(\alpha\):

\[
G_E = \int_{Dz_0} \left[ \prod_{\beta, a} \frac{d\lambda^{\beta,a} d\hat{\lambda}^{\beta,a}}{2\pi} \prod_{\beta, a} \Theta (\lambda^{\beta,a}) \exp \left( i \sum_{\beta, a} \lambda^{\beta,a} \hat{\lambda}^{\beta,a} - \frac{1}{2} \sum_{\beta, a} (\hat{\lambda}^{\beta,a})^2 \right) \times
\]

\[
\times \exp \left( -(q_2 - q_1) \sum_{\beta} \left( \sum_a \hat{\lambda}^{\beta,a} \right)^2 - \frac{(q_1 - q_0)}{2} \left( \sum_{\beta, a} \hat{\lambda}^{\beta,a} \right)^2 \right) \right]\]

\[
\times \exp \left( -iz_0 \sqrt{q_0} \sum_{\beta, a} \hat{\lambda}^{\beta,a} \right)^{\frac{m}{n}}
\]

\[(B24)\]
Performing two more Hubbard-Stratonovich transformations allows us to factorize over the relevant indices $\beta$ and $a$:

$$G_E = \int Dz_0 \left\{ \int Dz_1 \left[ \int Dz_2 H \left( A \left( z_0, z_1, z_2 \right) \right) \right]^m \right\}^m$$ (B25)

where

$$A \left( z_0, z_1, z_2 \right) = \frac{z_0 \sqrt{q_0} + z_1 \sqrt{q_1 - q_0} + z_2 \sqrt{q_2 - q_1}}{\sqrt{1 - q_2}}$$ (B26)

and we performed the Gaussian integral in $\lambda$, writing the definite Gaussian integral over $\lambda$ as an $H$ function, $H \left( x \right) = \int_x^{+\infty} Dz$. In the limit $n \to 0$ we get:

$$G_E = \frac{\log G_E}{n} = \frac{1}{m} \int Dz_0 \log \left( \int Dz_1 \left[ \int Dz_2 H \left( A \left( z_0, z_1, z_2 \right) \right) \right]^m \right)$$ (B27)

e. Final 1-RSB expression

Plugging eqs. (B21) and (B27) into eq. (B10) we obtain:

$$\langle \Omega \left( S, y \right)^n \rangle_{\{\xi^n\}} = \exp \left( -Nny \mathcal{F} \left( S, y \right) \right)$$

where we obtained an expression for eq. (B4):

$$\mathcal{F} \left( S, y \right) = - \left( \frac{m}{2} \hat{q}_0 \hat{q}_0 - \frac{y \left( m - 1 \right)}{2} q_1 \hat{q}_1 - \frac{y - 1}{2} q_2 \hat{q}_2 - \frac{\hat{q}_2}{2} \left( S \hat{S} + \frac{1}{y} G_S + \frac{\alpha}{y} G_E \right) \right)$$ (B28)

The order parameters are obtained by the saddle point equations. In order to study the zero-temperature limit $y \to \infty$, it is convenient to rearrange the terms as:

$$\mathcal{F} \left( S, y \right) = - \left( \frac{my}{2} \left( q_0 \hat{q}_0 - q_1 \hat{q}_1 \right) - \frac{y}{2} \left( q_2 \hat{q}_2 - q_1 \hat{q}_1 \right) - \frac{\hat{q}_2}{2} \left( 1 - q_2 \right) - S \hat{S} + \frac{1}{y} G_S + \frac{\alpha}{y} G_E \right)$$ (B29)

from which we see that in this limit the parameters must scale as:

$$m \to \frac{x}{y}$$

$$q_2 \to q_1 + \frac{\delta q}{y}$$

$$\hat{q}_2 \to \hat{q}_1 + \frac{\delta \hat{q}}{y}$$

giving, to the leading order in $y$:
\[ \mathcal{F}(S, \infty) = - \left( \frac{x}{2} (q_0 \hat{q}_0 - q_1 \hat{q}_1) - \frac{1}{2} (q_1 \delta \hat{q} + \hat{q}_1 \delta q) - \frac{\hat{q}_1}{2} (1 - q_1) - S \hat{S} + G_S^\infty + \alpha G_E^\infty \right) \]  

(B30)

where

\[ G_S^\infty = \frac{1}{x} \int Dz_0 \log \left( \int Dz_1 e^{x \hat{B}(z_0, z_1)} \right) \]  

(B31)

\[ \hat{B}(z_0, z_1) = \max_{z_2 \in \mathbb{R}, W \pm 1} \left( \tilde{A}^\infty (z_0, z_1, z_2; \tilde{W}) \right) \]  

(B32)

\[ \tilde{A}^\infty (z_0, z_1, z_2; \tilde{W}) = \frac{-z_2^2}{2} + \log \left( 2 \cosh \left( z_2 \sqrt{\delta q} + z_1 \sqrt{\hat{q}_1 - q_0} + z_0 \sqrt{q_0} + \tilde{S} \tilde{W} \right) \right) \]  

(B33)

\[ G_E^\infty = \frac{1}{x} \int Dz_0 \log \left( \int Dz_1 e^{x \hat{B}(z_0, z_1)} \right) \]  

(B34)

\[ B(z_0, z_1) = \max_{z_2} (A^\infty (z_0, z_1, z_2)) \]  

(B35)

\[ A^\infty (z_0, z_1, z_2) = -\frac{z_2^2}{2} + \log \left( H \left( \frac{z_0 \sqrt{q_0} + z_1 \sqrt{\hat{q}_1 - q_0} + z_2 \sqrt{\delta q}}{\sqrt{1 - \hat{q}_1}} \right) \right) \]  

(B36)

The expressions for \( G_S^\infty \) and \( G_E^\infty \) are obtained by the saddle point method, using \( y \to \infty \).

The resulting saddle point equations for the order parameters are:

\[ \hat{q}_0 = \frac{\alpha}{x \sqrt{\delta q}} \int Dz_0 \frac{\int Dz_1 e^{x \hat{B}(z_0, z_1)} z_E^* (z_0, z_1) \left( \frac{z_1}{\sqrt{\hat{q}_1 - q_0}} - \frac{z_0}{\sqrt{q_0}} \right)}{\int Dz_1 e^{x \hat{B}(z_0, z_1)}} \]  

(B37)

\[ \hat{q}_1 = \frac{\alpha}{\delta q} \int Dz_0 \frac{\int Dz_1 e^{x \hat{B}(z_0, z_1)} (z_E^* (z_0, z_1))^2}{\int Dz_1 e^{x \hat{B}(z_0, z_1)}} \]  

(B38)

\[ \delta \hat{q} = (1 - x) \hat{q}_1 + \frac{\alpha}{\sqrt{\delta q}} \int Dz_0 \frac{\int Dz_1 e^{x \hat{B}(z_0, z_1)} (z_E^* (z_0, z_1)) \left( \frac{z_1}{\sqrt{\hat{q}_1 - q_0}} - \frac{b(z_0, z_1)}{\sqrt{\delta q}} \right)}{\int Dz_1 e^{x \hat{B}(z_0, z_1)}} \]  

(B39)

\[ q_0 = \frac{1}{x \sqrt{\delta q}} \int Dz_0 \frac{\int Dz_1 e^{x \hat{B}(z_0, z_1)} z_S^* (z_0, z_1) \left( \frac{z_1}{\sqrt{\hat{q}_1 - q_0}} - \frac{z_0}{\sqrt{q_0}} \right)}{\int Dz_1 e^{x \hat{B}(z_0, z_1)}} \]  

(B40)

\[ q_1 = \frac{1}{\delta q} \int Dz_0 \frac{\int Dz_1 e^{x \hat{B}(z_0, z_1)} (z_S^* (z_0, z_1))^2}{\int Dz_1 e^{x \hat{B}(z_0, z_1)}} \]  

(B41)

\[ \delta q = (1 - x) q_1 - 1 + \frac{1}{\sqrt{\delta q}} \int Dz_0 \frac{\int Dz_1 e^{x \hat{B}(z_0, z_1)} z_S^* (z_0, z_1) \left( \frac{z_1}{\sqrt{\hat{q}_1 - q_0}} \right)}{\int Dz_1 e^{x \hat{B}(z_0, z_1)}} \]  

(B42)

\[ S = \frac{1}{\sqrt{\delta q}} \int Dz_0 \frac{\int Dz_1 e^{x \hat{B}(z_0, z_1)} z_S^* (z_0, z_1) \text{sign} \left( \hat{S} \left( z_1 \sqrt{\hat{q}_1 - q_0} + z_0 \sqrt{q_0} \right) \right)}{\int Dz_1 e^{x \hat{B}(z_0, z_1)}} \]  

(B43)
where
\[
\begin{align*}
    z^*_S (z_0, z_1) &= \arg\max_{z_2 \in \mathbb{R}} \left( \max_{W=\pm 1} \left( \tilde{A}^\infty (z_0, z_1, z_2; \tilde{W}) \right) \right) \\
    z^*_E (z_0, z_1) &= \arg\max_{z_2 \in \mathbb{R}} (A^\infty (z_0, z_1, z_2)) \\
    b (z_0, z_1) &= \frac{z^*_E (z_0, z_1)}{1 - q_1} \sqrt{\delta q} \left( z_0 \sqrt{q_0} + z_1 \sqrt{q_1} - q_0 + z^*_E (z_0, z_1) \sqrt{\delta q} \right)
\end{align*}
\]  

(B44)  
(B45)  
(B46)

The parameter \( x \) is implicitly set by the equation:
\[
\frac{1}{2} (q_0 \dot{q}_0 - q_1 \dot{q}_1) + \frac{\partial G^\infty_S}{\partial x} + \alpha \frac{\partial G^\infty_E}{\partial x} = 0
\]  
(B47)

where
\[
\begin{align*}
    \frac{\partial G^\infty_S}{\partial x} &= \frac{1}{x} \int D z_0 \left[ \int D z_1 e^{x \tilde{B}(z_0, z_1)} \tilde{B} (z_0, z_1) \right] - \frac{G^\infty_S}{x} \\
    \frac{\partial G^\infty_E}{\partial x} &= \frac{1}{x} \int D z_0 \left[ \int D z_1 e^{x B(z_0, z_1)} B (z_0, z_1) \right] - \frac{G^\infty_E}{x}
\end{align*}
\]  
(B48)  
(B49)

In this limit, and since we optimize over \( x \), \( \mathcal{F} (S, \infty) \) is equal to the local entropy \( \mathcal{I}_l \), i.e. the entropy of the solutions \( W \) (which has formally the role of an energy in our model). This is shown in Fig. 1. Note that the relationship between \( \mathcal{F} \) and \( \mathcal{I}_l \) is different from the one reported in the main text, eq. (6), because here we have used \( S \) directly as a control parameter rather than \( \gamma \) and thus no Legendre transform is required. The external entropy, i.e. the entropy of the reference configurations \( \tilde{W} \), is the sum of two terms in the 1-RSB scenario. The first, usually called complexity, accounts for the number of clusters of \( \tilde{W} \), and is implicitly set to zero by optimizing \( \mathcal{F} \) over \( x \) (see above). The second accounts for the number of configurations in each cluster (it is usually just called entropy, but here we need to qualify the name to avoid the confusion with the local entropy, which in our model has formally the role of an energy), and is computed from a first-order expansion in \( y \), since \( \mathcal{F} (S, y) = -\mathcal{I}_l - \frac{1}{y} \mathcal{F}_E \), giving:
\[
\begin{align*}
    \mathcal{I}_E &= \frac{1}{2} (-\delta \dot{q} - \delta q \dot{\delta q} + \delta \dot{q} \dot{q}_1 + \delta q \dot{q}_1) + C^\infty_S + \alpha C^\infty_E \\
    C^\infty_S &= -\frac{1}{2} \int D z_0 \left[ \int D z_1 e^{x \tilde{B}(z_0, z_1)} \log \left( 1 - \delta \dot{q} + z^*_S (z_0, z_1)^2 \right) \right] / \int D z_1 e^{x \tilde{B}(z_0, z_1)} \\
    C^\infty_E &= -\frac{1}{2} \int D z_0 \left[ \int D z_1 e^{x B(z_0, z_1)} \left( \log \left( 1 + z^*_E (z_0, z_1)^2 + b (z_0, z_1) \right) - b (z_0, z_1) \right) \right] / \int D z_1 e^{x B(z_0, z_1)}
\end{align*}
\]  
(B50)  
(B51)  
(B52)

In principle the external entropy should be non-negative since we are dealing with a model with discrete variables. Numerical evaluation of eq. (B50) gives negative results, indicating
that further steps of replica symmetry breaking are needed. However, the magnitude of the external entropy is very small ($\sim -10^{-6}$) and vanishes as $S \to 1$, therefore we expect that the corrections of further RSB steps would be very small and that the correct value of the external entropy would be 0 (see also the discussion in Sec. I A 3). The physical meaning of this result is that there is a sub-exponential number of configurations that can be defined as the center of the cluster, i.e. that yield the maximal local entropy at a given overlap, and that they are arranged in a sub-exponential number of distinct clusters.

3. Reference configurations energy and constrained case

a. Breaking the symmetry over reference configurations

The expression of eq. (B28) does not involve any overlaps relative to the reference configurations. However, we wish to compute the average energy associated with the reference configurations, which will involve such quantities (see below). Therefore, we need to preliminarily extract that information. To this end, we study a modified free energy with respect to eq. (B4):

$$F_C(S, y) = -\frac{1}{Ny} \langle \log \left( N C(S, y) \right) \rangle_{\{\xi^\mu\}}$$

$$= -\frac{1}{Ny} \left\langle \log \left( \sum_{\{\tilde{W}\}} f \left( \frac{1}{\sqrt{N}} \sum_i \tilde{W}_i \xi_i^\mu \right) \mathcal{N} \left( \tilde{W}, S \right)^y \right) \right\rangle_{\{\xi^\mu\}}$$

i.e. one in which an additional term $f \left( \frac{1}{\sqrt{N}} \sum_i \tilde{W}_i \xi_i^\mu \right)$ was included in the expression. If we set the function $f (x) = \Theta (x)$ we get the case in which the reference solutions $\tilde{W}$ are also constrained to be solutions to the classification problem. If we set it to some function of a parameter $\eta$ such that $\lim_{\eta \to 0} f (x) = 1$, we recover the previous case in the limit $\eta \to 0$, i.e. this amounts to introduce a symmetry-breaking term and then making it vanish at the end of the computation.

The computation follows along the lines of the previous case, but requires the introduction of some additional order parameters: $q^{\alpha \beta; \alpha' \beta'} = \frac{1}{\sqrt{N}} \tilde{W}^{\alpha \beta} \cdot \tilde{W}^{\alpha' \beta'}$ for the overlaps between reference configurations and $S^{\alpha \beta' ; \alpha \beta} = \frac{1}{\sqrt{N}} \tilde{W}^{\alpha \beta'} \cdot W^{\alpha \beta}$ for the overlaps between reference configurations and solutions. With the 1-RSB Ansatz, and including the constraint on the overlaps, we have:
\[ \tilde{q}_{\alpha\beta;\alpha'\beta'} = \begin{cases} 1 & \text{if } \alpha = \alpha', \beta = \beta' \\ \hat{q}_1 & \text{if } \alpha = \alpha', \beta \neq \beta' \\ \hat{q}_0 & \text{if } \alpha \neq \alpha' \end{cases} \] (B54)

\[ S_{\alpha'\beta';\alpha\beta} = \begin{cases} S & \text{if } \alpha = \alpha', \beta = \beta' \\ \hat{S}_1 & \text{if } \alpha = \alpha', \beta \neq \beta' \\ \hat{S}_0 & \text{if } \alpha \neq \alpha' \end{cases} \]

and analogous expressions for the conjugate parameters. The final expression for the free energy is:

\[
\mathcal{F}_C (S, y) = - \left( \frac{m}{2y} (\hat{q}_0 \hat{q}_0 - \hat{q}_1 \hat{q}_1) - \frac{1}{2y} \hat{q}_1 (1 - \hat{q}_1) + \frac{my}{2} (q_0 \hat{q}_0 - q_1 \hat{q}_1) + \frac{y}{2} (q_2 \hat{q}_2 - q_1 \hat{q}_1) - \frac{\hat{q}_2}{2} (1 - q_2) - \left( \hat{S} \hat{S} - \hat{S}_1 \hat{S}_1 \right) \right) + m \left( \hat{S}_0 \hat{S}_0 - \hat{S}_1 \hat{S}_1 \right) + \frac{1}{y} \frac{G_{CS}}{y} + \frac{\alpha}{y} G_{CE} \right) \] (B55)

where

\[
G_{CS} = \frac{1}{m} \int D\hat{z}_0 \int D\hat{z}_0 \log \left( \int D\hat{z}_1 \int D\hat{z}_1 \left[ \sum_{W=\pm 1} e^{\hat{W} K(\hat{z}_0, z_0, \hat{z}_1, z_1)} \right] \right) \] (B56)

\[
\hat{A}_C (z_0, z_1, z_2; \hat{W}) = z_2 \sqrt{\hat{q}_2 - \hat{q}_1} + z_1 \sqrt{\hat{q}_1 - \hat{q}_0} + z_0 \sqrt{\hat{q}_0} + \left( \hat{S} - \hat{S}_1 \right) \hat{W} \] (B57)

\[
K (\hat{z}_0, z_0, \hat{z}_1, z_1) = \hat{z}_1 \sqrt{\left( \hat{q}_1 - \hat{q}_0 \right) - \frac{(\hat{S}_1 - \hat{S}_0)^2}{\hat{q}_1 - \hat{q}_0}} + z_1 \frac{\hat{S}_1 - \hat{S}_0}{\sqrt{\hat{q}_1 - \hat{q}_0}} \] (B58)
\[ G_{CE} = \frac{1}{m} \int Dz_0 \int Dz_0 \log \left( \int D\tilde{z}_1 \int Dz_1 \left[ \int Dz_2 H(A(z_0, z_1, z_2)) \right] \right) \times (B59) \]
\[ L(\tilde{z}_0, z_0, \tilde{z}_1, z_1, z_2) = \int D\tilde{\lambda} f \left( \frac{z_2 S_0 - \tilde{S}_0}{\sqrt{1-q_1}} + \lambda \sqrt{\frac{(q_2 - q_1) - \frac{(s-S_1)}{1-q_1}}{q_2 - q_1}} + z_1 \frac{\tilde{S}_1 - \tilde{S}_0}{\sqrt{q_1 - q_0}} + \right) \]
\[ + z_0 \frac{\tilde{S}_0}{\sqrt{q_0}} + \tilde{z}_1 \left( \tilde{q}_1 - \tilde{q}_0 \right) - \frac{\left( \tilde{S}_1 - \tilde{S}_0 \right)^2}{q_1 - q_0} + \tilde{z}_0 \left[ \tilde{q}_0 - \frac{(\tilde{S}_0)^2}{q_0} \right] \]

From these expression, we can note that the dependency on the function \( f \) only enters the equations through the expression of \( L \) in \( G_{CE} \). Also, this expression does not depend on \( y \). This has two consequences:

1. In the case where \( \lim_{\eta \to 0} f(x) = 1 \), \( G_{CE} \to G_E \), i.e. the expression does not depend any more on \( q_1, \tilde{q}_0, \tilde{S}_1 \) or \( \tilde{S}_0 \) and simplifies to the previous case, as expected. In turn, this implies that the conjugate order parameters \( \hat{q}_1, \tilde{q}_0, \hat{S}_1 \) and \( \tilde{S}_0 \) all tend to 0, thus reducing the expression of the free energy to the previous case eq. (B28);

2. In the limit \( y \to \infty \) in the constrained case \( (f(x) = \Theta(x)) \), we also have \( G_{CE} \to G_E \), since the term with \( y \) in the exponent dominates the saddle point expansion. Again we recover expression (B28) for the free energy of the system, which means that the local entropy is unchanged in the constrained case. This may suggest that, even in the unconstrained case, the reference configuration \( \tilde{W} \) is never “too far” from an actual solution to the problem (more precisely, within a distance \( o(N) \) from a solution). Note, however, that — as one would expect — the external entropy is different in this case, since it depends on the first order expansion in \( y \), which is affected by the \( L \) term.

Following observation 1, we can derive the expression for the order parameters \( \tilde{q}_1, \tilde{q}_0, \tilde{S}_1 \) and \( \tilde{S}_0 \) by using the saddle point equations and by assuming that the conjugate parameters \( \hat{q}_1, \tilde{q}_0, \tilde{S}_1 \) and \( \tilde{S}_0 \) are of order \( \eta \ll 1 \) and taking the leading order in the resulting expression.
We actually only need the results for $\tilde{S}_1$ and $\tilde{S}_0$, which turn out to be:

$$\tilde{S}_1 = \frac{S}{1 - m} + \frac{1}{y(m - 1)\sqrt{q_1 - q_0}} \int Dz_0 \frac{I_{d_1}(z_0)}{I_s(z_0)}$$ (B61)

$$\tilde{S}_0 = \frac{1}{my} \left( \frac{1}{\sqrt{q_1 - q_0}} \int Dz_0 \frac{I_{d_1}(z_0)}{I_s(z_0)} - \frac{1}{\sqrt{q_0}} \int Dz_0 z_0 \frac{I_d(z_0)}{I_s(z_0)} \right)$$ (B62)

$$I_s(z_0) = \int Dz_1 \left[ \int Dz_2 \sum_{W = \pm 1} \left( 2 \cosh \left( \tilde{A} \left( z_0, z_1, z_2; \tilde{W} \right) \right) \right)^y \right]^{m-1}$$ (B63)

$$I_d(z_0) = \int Dz_1 \left[ \int Dz_2 \sum_{W = \pm 1} \left( 2 \cosh \left( \tilde{A} \left( z_0, z_1, z_2; \tilde{W} \right) \right) \right)^y \right] \times$$ (B64)

$$I_{d_1}(z_0) = \int Dz_1 \left[ \int Dz_2 \sum_{W = \pm 1} \left( 2 \cosh \left( \tilde{A} \left( z_0, z_1, z_2; \tilde{W} \right) \right) \right)^y \right] \times$$ (B65)

$$\times \left( \int Dz_2 \sum_{W = \pm 1} \tilde{W} \left( 2 \cosh \left( \tilde{A} \left( z_0, z_1, z_2; \tilde{W} \right) \right) \right)^y \right)^{m-1}$$

In the limit $y \to \infty$, we have the scaling:

$$\tilde{S}_1 = \frac{S - \delta S}{y}$$

and finally the expressions:

$$\delta S = \frac{1}{\sqrt{q_1 - q_0}} \int Dz_0 \int Dz_1 z_1 e^{x \tilde{B}(z_0, z_1)} \tilde{W}^*(z_0, z_1) - xS$$ (B66)

$$\tilde{S}_0 = \frac{1}{x\sqrt{q_1 - q_0}} \int Dz_0 \int Dz_1 z_1 e^{x \tilde{B}(z_0, z_1)} \tilde{W}^*(z_0, z_1) +$$ (B67)

$$- \frac{1}{x\sqrt{q_0}} \int Dz_0 z_0 \int Dz_1 e^{x \tilde{B}(z_0, z_1)} \tilde{W}^*(z_0, z_1)$$

where

$$\tilde{W}^*(z_0, z_1) = \arg\max_{\tilde{W} = \pm 1} \left( \max_{z_2 \in \mathbb{R}} \left( \tilde{A}^\infty \left( z_0, z_1, z_2; \tilde{W} \right) \right) \right)$$ (B68)

### b. Energy density

In order to compute the typical energy density of the unconstrained reference configurations $\tilde{W}$, we need to evaluate the probability of classifying incorrectly a pattern $\xi^*$ drawn at random from the training set. This probability can be obtained by calculating:
\[ P(\sigma^{*} \neq 1) = \left\langle \Theta \left( -\frac{1}{\sqrt{N}} \sum_{i} \tilde{W}_i \xi_i^{*} \right) \right\rangle_{\tilde{W}} \]  

(B69)

where the average is defined over the weighted measure \( d\mu_{\tilde{W}} (\tilde{W}) = d\mu (\tilde{W}) N_{\xi} (\tilde{W}, S)^{y}. \)

Since:

\[
\left\langle \prod_{\mu} \Theta \left( -\frac{1}{\sqrt{N}} \sum_{i} \tilde{W}_i \xi_i^{*} \right) \right\rangle_{\tilde{W}} = \frac{\int d\mu_{\tilde{W}} (\tilde{W}) \prod_{\mu} \Theta \left( -\frac{1}{\sqrt{N}} \sum_{i} \tilde{W}_i \xi_i^{\mu} \right)}{\int d\mu_{\tilde{W}} (\tilde{W})} \]  

(B70)

this calculation can be carried out straightforwardly by exploiting the replica trick, i.e. by rewriting the ratio in (B70) as:

\[
\lim_{n \to 0} \int d\mu_{\tilde{W}} (\tilde{W}) \Theta \left( -\frac{1}{\sqrt{N}} \sum_{i} \tilde{W}_i \xi_i^{*} \right) \left( \int d\mu_{\tilde{W}} (\tilde{W}) \right)^{n-1} = \]  

\[
= \lim_{n \to 0} \int \prod_{c} d\mu_{\tilde{W}} (\tilde{W}^{c}) \Theta \left( -\frac{1}{\sqrt{N}} \sum_{i} \tilde{W}_i^{1} \xi_i^{*} \right) \]  

(B71)

where we have introduced \( n - 1 \) unconstrained replicas of the reference solution, leaving out the replica index 1 for the \( \tilde{W} \)-replica coupled to the pattern \( \xi^{*} \) by the constraint. In this way the quenched disorder can be averaged out, and in the \( n \to 0 \) limit one recovers the initial expression.

As noted in the previous section, when one extracts the overlaps referred to the reference configurations by introducing vanishing constraints (i.e. when \( \eta \to 0 \)), the conjugate parameters related to these overlaps tend to vanish as well.

Therefore, if one organizes the calculation similarly to the previous ones, it is easy to see that in (B71) the entropic terms cancel out and the only non-zero contribution to the average comes from the energetic part \( G'_{E} \), where:
\[ G'_E = \int \frac{d\tilde{\lambda}^1}{2\pi} \prod_{\alpha\beta} \frac{d\tilde{\lambda}^{\alpha\beta}}{2\pi} \Theta (-\tilde{\lambda}^1) \prod \Theta (\tilde{\lambda}^{\alpha\beta}) \times \]
\[ \times \exp \left( i \left( \tilde{\lambda}^1 + \sum_{\alpha\beta} \tilde{\lambda}^{\alpha\beta} \tilde{\lambda}^{\alpha\beta} \right) - \frac{1}{2} \left( \tilde{\lambda}^1 \right)^2 + \sum_{\alpha\beta} (\tilde{\lambda}^{\alpha\beta})^2 \right) \times \]
\[ \times \exp \left( -q_1 \sum_{a > b} \tilde{\lambda}^{\alpha\beta} \tilde{\lambda}^{\alpha\beta} \right) \times \]
\[ \times \exp \left( -q_0 \sum_{a > a', \beta' b} \tilde{\lambda}^{\alpha\beta} \tilde{\lambda}^{\alpha\beta} \right) \times \]
\[ \times \exp \left( -\sum_{\beta} \sum_{a} \tilde{\lambda}^1 \tilde{\lambda}^{1\beta} \left( \tilde{S}_1 - \tilde{S}_0 \right) - \sum_{\alpha\beta} \sum_{a} \tilde{\lambda}^1 \tilde{\lambda}^{\alpha\beta} \tilde{S}_0 \right) \]  

\[ (B72) \]

The final expression we obtain is the following:

\[ P (\sigma^* \neq 1) = \int_{Dz_0} \frac{\int_{Dz_1} \left( \int_{Dz_2} H (A (z_0, z_1, z_2))^{y} \right)^{m-1} \int_{Dz_2} H (A (z_0, z_1, z_2))^{y} H (-C (z_0, z_1, z_2))}{\int_{Dz_1} \left( \int_{Dz_2} H (A (z_0, z_1, z_2))^{y} \right)^{m}} \]

\[ \text{with the definition (B26), and where:} \]

\[ C (z_0, z_1, z_2) = \frac{z_0 \frac{\tilde{S}_0}{\sqrt{q_0}} + z_1 \frac{\tilde{S}_1 - \tilde{S}_0}{\sqrt{q_1 - q_0}} + z_2 \frac{S - \tilde{S}_1}{\sqrt{q_2 - q_1}}}{\sqrt{1 - \frac{S}{q_0} - \frac{(S - \tilde{S}_1)^2}{q_1 - q_0} - \frac{(S - \tilde{S}_1)^2}{q_2 - q_1}}} \]

In the limit \( y \to \infty \), we have:

\[ \int_{Dz_1} e^{x B(z_0, z_1)} H \left( -\frac{z_0 \frac{\tilde{S}_0}{\sqrt{q_0}} + z_1 \frac{\tilde{S}_1 - \tilde{S}_0}{\sqrt{q_1 - q_0}} + z_2 \frac{S - \tilde{S}_1}{\sqrt{q_2 - q_1}}}{\sqrt{1 - \frac{S}{q_0} - \frac{(S - \tilde{S}_1)^2}{q_1 - q_0} - \frac{(S - \tilde{S}_1)^2}{q_2 - q_1}}} \right) \]

\[ \text{which is shown in Fig. 2} \]

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[26] we should have used a Kronecker delta symbol here, but this abuse of notation comes in handy since in the following we will use integrals instead of sums for the weights.