Optimization Problems and Algorithms from Computer Science

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Article Outline

Glossary

Combinatorial optimization The search for an optimal configuration in terms of a cost function on a discrete set of allowed configurations.

Ground state The configuration of a model for a physical system of many interacting degrees of freedom described by a Hamiltonian or energy function that has the lowest energy. Also dented as the global minimum of the energy of the system.

Disordered system A physical system with frozen in or quenched inhomogeneities, usually modeled by an energy function containing parameters that are random numbers obeying in prescribed probability distribution.

Universal properties Properties that do not depend on microscopic details of a physical system, like the critical exponents at a continuous phase transition or fractal dimensions.

Network flows A function defined on the edges of a graph that obeys mass balance constraints at each node. A number of polynomial optimization problems relevant for disordered systems can be formulated as network flow models.

Definition of the Subject and its Importance

Optimization problems in statistical physics occur whenever the ground state of a classical model for a complex condensed matter system has to be determined, which is necessary for understanding its. low temperature properties. In some cases calculating the ground state is an easy task as for instance for the paradigmatic model for a ferromagnet: The configuration of all magnetic moments or spins with the lowest energy is the one, where all spins point in the same direction. But usually the situation is much more complex and the problem of calculating the state with the lowest energy is highly non-trivial. This occurs typically in systems with quenched disorder and/or frustration, which means that their Hamiltonian or energy function consists of competing terms that cannot be satisfied simultaneously. Powerful algorithms from computer science have been devised to find the optimum of complex cost-functions and in some cases this can even be achieved in polynomial time. In recent years many of these algorithms could be successfully applied to physically relevant model systems: to polymers in random media, interface problems in random ferromagnets, magnetic flux-lines in disordered environments, spin glasses, and many more.

Introduction

Solid materials which contain a substantial degree of quenched disorder, so called disordered systems, have been an experimental and a theoretical challenge for physicists for many decades. The different thermodynamic phases emerging in random magnets, the aging properties and memory effects of spin glasses, the disorder induced conductor-to-insulator transition in electronic or bosonic systems, the collective behavior of magnetic flux lines in amorphous high temperature superconductors, and the roughening transition of a disordered charge density wave systems are only a few examples for these fascinating phenomena that occur due to the presence of quenched disorder.

Analytic studies of models for these systems are usually based on perturbation theories valid for weak disorder, on phenomenological scaling pictures or on mean-field approximations. Therefore the demand for efficient numerical techniques that allow the investigation of the model Hamiltonians of disordered systems has always been high. Three facts make life difficult here: 1) The regime, where disorder effects are most clearly seen, are at low temperatures – and are even best visible at zero temperature; 2) the presence of disorder slows the dynamics of theses systems down, they become *glassy*, such that for instance conventional Monte-Carlo or molecular dynamics simulations encounter enormous equilibration problems; 3) any numerical computation of disordered systems has to incorporate an extensive disorder average.

In recent years more and more model systems with quenched disorder were found that can be investigated numerically 1) at zero temperature, 2) without equilibration problems, 3) extremely fast, in polynomial time (for reviews see [1,2,3]). This *is* indeed progress, which became possible by the application of *exact* combinatorial optimization algorithms developed by mathematicians and computer scientists over the last few decades. This gift is not for free: first a mapping of the problem of finding the *exact* ground state of the model Hamiltonian under consideration onto a standard combinatorial optimization problem has to be found. If one is lucky, this problem falls into the class of P-problems, for which polynomial algorithms exist. If not, the intellectual challenge for the theoretical physicist remains to reformulate the model Hamiltonian in such a way that its universality class is not changed but a mapping on a P-problem becomes feasible.

An optimization problem can be described mathematically in the following way: let $\underline{\sigma} = (\sigma_1, \ldots, \sigma_n)$ be a vector with n elements which can take values from a domain $X^n : \sigma_i \in X$. The domain X can be either discrete, for instance $X = \{0, 1\}$ or $X = Z$ the set of all integers (in which case it is an integer optimization problem) or X can be continuous, for instance $X = R$ the real numbers. Moreover, let $\mathcal{H}$ be a real valued function, the cost function or objective, or in physics usually the Hamiltonian or the energy of the system. The *minimization problem* is then:

$$\text{Find } \underline{\sigma} \in X^n, \text{ which minimizes } \mathcal{H}\,!$$

A maximization problem is defined in an analogous way. It is sufficient to consider only minimization problems, since maximizing a function H is equivalent to minimizing $-H$. Minimization problems in which the set X is *countable* are called *combinatorial* [4,5,6]. Optimization methods for real valued variables are treated mainly in mathematical literature and in books on numerical methods, see e. g. [8].

Constraints, must hold for the solution, may be expressed by additional equations or inequalities. An arbitrary value of $\underline{\sigma}$, which fulfills all constraints, is called *feasible*. Usually constraints can be expressed more conveniently without giving equations or inequalities. A famous example is the Traveling Salesman Problem (TSP) [7].

The TSP has attracted the interest of physicist several times. For an introduction, see [9]. The model is briefly presented here. Consider n cities distributed randomly in a plane. Without loss of generality the plane is considered to be the unit square. The minimization task is to find the shortest round-tour through all cities which visits each city only once. The tour stops at the city where it started. The problem is described by

$$X = \{1, 2, \ldots, n\} \tag{1}$$

$$H(\underline{\sigma}) = \sum_{i=1}^{n} d(\sigma_i, \sigma_{i+1}) \tag{2}$$

where $d(\sigma_\alpha, \sigma_\beta)$ is the distance between cities σ_α and σ_β and $\sigma_{n+1} \equiv \sigma_1$. The constraint that every city is visited only once can be realized by constraining the vector $\underline{\sigma}$ to be a permutation of the sequence $[1, 2, \ldots, n]$.

The optimum order of the cities for a TSP depends on their exact positions, i. e. on the random values of the distance matrix d. It is a feature of all problems we will encounter here that they are characterized by various random parameters. Each random realization of the parameters is called an *instance* of the problem. In general, if we have a collection of optimization problems of the same (general) type, we will call each single problem an instance of the general problem.

Because the values of the random parameters are fixed for each instance of the TSP, one speaks of *frozen* or *quenched* disorder. To obtain information about the general structure of a problem one has to average measurable quantities, like the length of the shortest tour for the TSP, over the disorder.

In this article we give an overview of *methods* how to *solve* these problems, i. e. how to find the optimum. Interestingly, there is no single way to achieve this. For some problems it is very easy while for others it is rather hard, this refers to the time you or a computer will need at least to solve the problem, it does not say anything about the elaborateness of the algorithms which are applied. Additionally, within the class of hard or within the class of easy problems, there is no universal method. Usually, even for each kind of problem there are many different ways to obtain an optimum. Once a problem becomes large, i. e. when the number of variables n is large, it is impossible to find a minimum by hand. Then computers are used to obtain a solution. Only the rapid development in the field of computer science during the last two decades has pushed forward the application of optimization methods to many problems from science and real life.

We will review some of the most fruitful applications of polynomial algorithms from the realm of combinatorial optimization to various problems in the statistical physics of disordered systems. The next section presents the application of Dijkstra's algorithm for finding shortest paths in weighted networks to the model of a non-directed polymer in a disordered environment with isotropical correlations. Then, in the 4th and 5th section, we discuss minimum cost flow problems on weighted graphs and its solution via the

successive shortest path algorithm and apply it to the entanglement transition of elastic lines in a disordered environment and to the loop percolation transition in a vortex glass model. In the 6th section we focus on the minimum cut-maximum flow problem and discuss among its many applications the roughening transition of elastic media in a disordered environment. The 7th section is devoted to the random field Ising model and how its ground states can be computed with maximum-flow-minimum-cut techniques. The spin glass problem is presented in the 8th section with a mapping onto minimum weighted matching in two dimensions and a brief outline of branch and cut methods for the higher dimensional case. The 9th section is devoted to finite temperature properties of the random bond Potts model and how its free energy can be computed in the limit of infinite Potts states. An outlook in the 10th section closes this chapter.

Polymers in a Disordered Environment

A well studied model of a single elastic line [10], like an individual polymer or a single magnetic flux line in a type-II superconductor, in a disordered environment is the following: If one excludes overhangs (and by this also self-overlaps) of the elastic lines one can parametrize its configuration by the longitudinal coordinate z. The line configuration can then be described by the transverse coordinate $\mathbf{r}(z)$ as a function of z. The presence of disorder is usually modeled by a random potential energy $V(\mathbf{r}, z)$ and the ground state configuration of the line is highly nontrivial due to the competition between the elastic energy, that tends to straighten the line, and the random energy, that tries to bend the line into positions of favorable energy:

$$\begin{aligned}\mathcal{H}_{\text{single-line}} &= \mathcal{H}_{\text{elastic}} + \mathcal{H}_{\text{random}} \\ &= \int_0^H \mathrm{d}z \left\{ \frac{\gamma}{2} \left[\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}z} \right]^2 + V[\mathbf{r}(z), z] \right\} , \end{aligned} \tag{3}$$

where H is the longitudinal length (not the proper length) of the line. The random potential energy is a Gaussian variable with prescribed mean and correlations $\langle\langle V[\mathbf{r}, z] V[\mathbf{r}', z']\rangle\rangle = g(\mathbf{R} - \mathbf{R}')$, where $\mathbf{R} = (\mathbf{r}, z)$ and $\langle\langle\cdots\rangle\rangle$ denotes the average over the disorder.

A lattice version of this continuum model is the *directed* polymer model: The lines correspond to directed paths on a hyper-cubic lattice that start at a specific lattice site, say $(0, 0, \ldots, 0)$ and proceed only in the $(1, 1, \ldots, 1)$ direction along the bonds. The energy contribution for a path passing bond $\mathbf{i}$ of the lattice is a *positive* random variable $e_\mathbf{i}$ and the total energy of a path $\mathcal{P}$ is simply

$$\mathcal{H}^{\text{lattice}}_{\text{single-line}} = \sum_{\mathbf{i}\in\mathcal{P}} e_\mathbf{i} = \sum_{\mathbf{i}} e_\mathbf{i} n_\mathbf{i} , \tag{4}$$

where $n_\mathbf{i} = 1$ if the path passes bond $\mathbf{i}$ (i. e. $\mathbf{i} \in \mathcal{P}$) and $n_\mathbf{i} = 0$ otherwise.

One is interested in isotropically correlated disorder and consider the problem on a *non-directed* (square) lattice (i. e. paths can pass any bond in both directions) in order not too exclude overhangs right from the beginning. In case of uncorrelated disorder overhangs were shown to be irrelevant [12], but for isotropically correlated disorder this is not clear. The latter is defined to decay algebraically with the spatial distance of the bonds

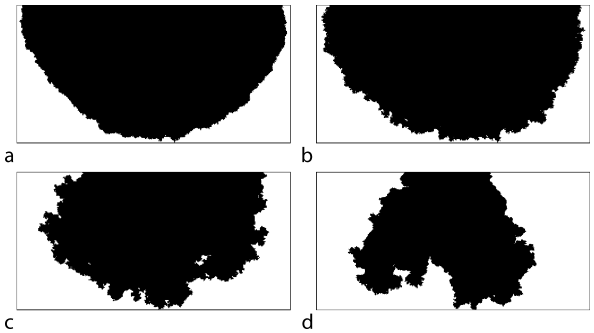
$$\langle\langle e_\mathbf{i} - e_\mathbf{j}\rangle\rangle = |\mathbf{R}_\mathbf{i} - \mathbf{R}_\mathbf{j}|^{2\alpha-1} , \tag{5}$$

where $\mathbf{R}_\mathbf{i}$ spatial position of bond $\mathbf{i}$ and α is the correlation exponent: Note that one expects short-range correlations like $\langle\langle e_\mathbf{i} - e_\mathbf{j}\rangle\rangle \propto \exp(-|\mathbf{R}_\mathbf{i} - \mathbf{R}_\mathbf{j}|/\lambda)$ with a finite correlation length λ, to be irrelevant and only long-range correlations like (5) to change the universality class of the system. Increasing α imply stronger correlations, uncorrelated disorder corresponds to $\alpha \to -\infty$. The kind of correlated disorder described by (5) can be realized by generating correlated random numbers are generated using a well-established numerical procedure [11].

Exact ground states of the Hamiltonian (4) or optimal paths are calculated using Dijkstra's algorithm (note that all energies $e_\mathbf{i}$ are positive). This simple polynomial algorithm works as follows: Let $V = \{1, \ldots, L^d\}$ be the set of lattice sites and $A = \{(i, j) | i, j \in V \text{ nearest neighbors}\}$ the set of bonds. The algorithm increases successively a subset S of sites for which the optimal path starting at the fixed site s are known. Obviously initially $S := \{s\}$. We denote the energy of the optimal path starting at s and terminating at i with $E(i)$ and since all optimal paths can be constructed via a predecessor list, we keep track of this list, too, via an array pred(i), denoting the predecessor site of site i in a **shortest path** from s to i:$$

algorithm Dijkstra
begin
  $S := \{s\}$; $\overline{S} := V \backslash \{s\}$;
  $E(s) := 0$, pred$(s) := 0$;
  while $|S| < |V|$ **do**
  begin
    choose (i, j): $E(j) := \min_{k,m}\{E(k)$
      $+ e_{(k,m)} | k \in S, m \in \overline{S}, (k, m) \in A\}$;
    $\overline{S} := \overline{S} \backslash \{j\}$; $S := S \cup \{j\}$;
    pred$(j) := i$;
  end
end

In Fig. 1 we show examples of the set $\{i\}$ of lattice sites that are end-points of optimal paths starting from a fixed initial



Optimization Problems and Algorithms from Computer Science, Figure 1
Example for the growth front of the non-directed polymer for uncorrelated disorder (a and b) and correlated disorder (c and d; $\alpha = 0.4$). The *black pixels* indicate the lattice sites of the (square) lattice are connected via optimal paths to the offspring (center of the top line) with energy less than a given value (from [13])

site and having a total energy $E(i)$ less than a given value $E_{\max}$. For uncorrelated disorder the surface of this set is roughly a semi-circle, whereas for strongly correlated disorder the surface becomes topologically more complicated.

The universal properties of the optimal paths are typically described the scaling of two characteristic quantities: The average transverse fluctuations $\langle\langle \mathbf{r}^2 \rangle\rangle$ and the average energy fluctuations $\langle\langle E^2 \rangle\rangle$. Both are expected to grow algebraically with the the longitudinal distance H between starting point and end point of the paths:

$$\langle\langle \mathbf{r}^2 \rangle\rangle \propto H^{\nu} \quad \text{and} \quad \langle\langle E^2 \rangle\rangle \propto H^{\omega} \,, \tag{6}$$

where ν is called the roughness exponent and ω the energy fluctuation exponent. For uncorrelated disorder ($\alpha \to -\infty$) one knows $\nu = 2/3$ and $\omega = 1/3$. By computing the optimal paths for several thousands of samples for a given disorder correlation exponent α and for a given longitudinal distances H and fitting the resulting data for transverse and energy fluctuations to the expected power laws we can extract the exponents ν and ω (for details see [13]). The resulting estimates in 2d show that the correlations are relevant for $\alpha > 0$ and the roughness exponent increases linearly for $\alpha > 0$ from its value for uncorrelated disorder $\nu = 2/3$. Although the number of overhangs in the optimal paths we computed in the non-directed case increased with α (i. e. increasing correlations) the fraction of bonds contributing to overhangs scaled to zero for all values of α we considered. Hence overhangs appear to be irrelevant also in the presence of correlated disorder.

Many Repulsive Elastic Lines in Random Media

When one puts interacting elastic lines together into a finite system with a given density of lines they will show interesting collective behavior. Examples are the entanglement of magnetic flux lines in high-T_c superconductors in the mixed phase [14] or the entanglement of polymers in materials like rubber [15]. The degree of entanglement of the lines usually manifests itself in various measurable properties like stiffness or shear modulus in the case of polymers and in transport or dynamical properties for magnetic flux lines in superconductors. A theoretical description of these line systems can be based on the single-line Hamiltonian (3) plus an appropriate line interaction term:

$$\mathcal{H}_{\text{many-lines}} = \sum_{i=1}^{N} \mathcal{H}^{(i)}_{\text{single-line}} + \sum_{i<j} \int_0^L \mathrm{d}z \int_0^L \mathrm{d}z' \; V_{\text{int}}[\mathbf{R}_i(z) - \mathbf{R}_j(z')] \,, \tag{7}$$

where $\mathbf{R}_i(z) = (\mathbf{r}_i(z), z)$ is the spatial position of the infinitesimal line segment $\mathrm{d}z$ of the ith line. If the interactions $V_{\text{int}}[\mathbf{R}_i(z) - \mathbf{R}_j(z')]$ are short ranged (i. e. in case of flux lines the screening length small compared to the average line distance) or just hard core repulsive, and the random, δ-correlated disorder potential $V_r[\mathbf{r}_i(z), z]$ in (3) is strong compared to the elastic energy ($\propto \gamma$) this continuum model reduces to a lattice model reminiscent of the single-line lattice model (4):

$$\mathcal{H}^{\text{lattice}}_{\text{many-lines}} = \sum_{\mathbf{i}} e_{\mathbf{i}} n_{\mathbf{i}} \,, \tag{8}$$

where $n_{\mathbf{i}} = 1$ if a line passes bond $\mathbf{i}$ and $n_{\mathbf{i}} = 0$ otherwise and the *positive* random variable $e_{\mathbf{i}}$ is the energy cost for a line segment to occupy bond $\mathbf{i}$. The hard core constraint is thus enforced on the bonds but for the sake of an easier formal description we allow the lines to touch in isolated points, the lattice sites. The lines live on the bonds of a simple cubic lattice with a lateral width L and a longitudinal height H ($L \times L \times H$ sites) with free boundary conditions in all directions. Each line starts and ends at an arbitrary position on the bottom respective top planes. The number N of lines threading the sample is fixed by a prescribed density $\rho = N/L^2$. For a single line $N = 1$, one recovers the non-directed polymer model (4). The random bond energies are uniformly distributed over the interval $[0, 1]$.

Note that the allowed configurations of the bond variables $n_{\mathbf{i}}$ are only those that can be identified with lines threading the samples (or loops inside the sample, which, however, cost energy and therefore do not occur in the

ground state), which means that the number of occupied bonds connected to a lattice site that lies neither on the top nor on the bottom plane has always to be even. If we connect all sites on the top to an extra site, called the source, an all sites on the bottom to another extra site, called the target, than the latter statement remains true also for the top an bottom plane. We can now say that N lines start at the source node and terminate at the target node, or, in network flow jargon: The feasible configurations of the variables $n_{\mathbf{i}}$ constitute a flow with zero excess on all lattice sites and an excess $+N$ and $-N$ for the source and target node, respectively.

Thus the determination of the ground state configuration of the N-line problem with the Hamiltonian (8) is a **minimum-cost-flow-problem**, which can be solved with a successive shortest path algorithm [1,2,3]. In essence one starts with the zero flow $n_{\mathbf{i}} = 0$, corresponding to zero lines in the system, and sends successively one unit of flow from the source to the target, corresponding to adding one line after the other to the system. This has to happen with the minimal energy, i. e. along optimal paths, which are calculated using Dijkstra's algorithm that we encountered already in the single line problem discussed in the last section. However, when trying to add a line to a system with a number, say M, of lines already present, the existing line configuration sometimes must be changed to minimize the total energy for $M+1$ line solution. That becomes feasible by allowing flow to be sent *backwards* on already occupied bonds. By this operation one *gains* energy (whereas occupying an empty bond $\mathbf{i}$ always costs energy $e_{\mathbf{i}} \geq 0$), which means one has to operate on a network that has to be adapted to the existing flow configuration and has negative energies on all occupied bonds. Unfortunately Dijkstra's algorithm works only for positive bond energies, and one has either to use a slower (label-correcting) algorithm to find the optimal paths in a graph with negative edge costs [3] or one has to use the concept of node potentials, by which one can make all energies in the adapted network non-negative without changing the actual shortest paths. This procedure is described in full detail in [3].

The resulting line configuration is then analyzed. One computes the winding angle of all line pairs as indicated in Fig. 2 (c.f. [16]). For each z-coordinate the vector connecting the two lines is projected onto that basal plane (*left* part of Fig. 2). $z = 0$ gives the reference line with respect to which the consecutive vectors for increasing z-coordinate have an angle $\phi(z)$. If the two lines intersect one neglects the intersection point and interpolate between the last and the next point in such a way that the global winding angle is minimized. One defines two lines to be *entangled* when $\phi(z) > 2\pi$. This choice is one that measures entanglement from the topological perspective [17], and comes from the requirement that an entangled pair of lines can not be separated by a suitable linear transformation in the basal plane (i. e. the lines almost always would cut each other, if one were shifted). The precise definition of entanglement is not of major relevance, and the one used is useful since it is the computationally easiest.

Sets or *bundles* of pairwise entangled lines are formed so that a line belongs to a bundle if it is entangled at least with one other line in the set. The topological multi-line-entanglement could be characterized by other measures as well; the universal properties of the transition will not depend on these. These line bundles are spaghetti-like – i. e. topologically complicated and knotted sets of one-dimensional objects. To study the size distribution of these objects one projects these bundles on the basal plane, as indicated in Fig. 2, where a bundle projects onto a connected cluster. The probability for two lines to be entangled increases with increasing system height. Consequently one would expect that the bundle size increases with H, and therefore also their projections, the clusters. This scenario is exemplified in Fig. 3, for the largest height the largest cluster spans from one side of the system to the other, i. e. it *percolates*.

Hence, for a given line density ρ one expect that for system heights larger than a critical value H_c an system spanning large entangled bundle occurs, containing an infinite number of lines in the limit $L \to \infty$. One calls this an *entanglement transition* occurring at a finite system height H_c. In the projection plane this appears like a percolation transition and in [18] it was shown that this transition is in the same universality class as conventional bond percolation.

Vortex Glasses and Loop Percolation

Another application of the successive shortest path algorithm for minimum-cost-flow-problems is finding the ground state of the Hamiltonian

$$H = \sum_{\mathbf{i}} (n_{\mathbf{i}} - b_{\mathbf{i}})^2 \quad \text{with the constraint} \quad \forall k: \sum_{l \text{ n.n. of } k} n_{(kl)} = 0\,, \tag{9}$$

where the integer variables $n_{\mathbf{i}}$ live on the bonds $\mathbf{i}$ of a d-dimensional hyper-cubic lattice and $b_{\mathbf{i}} \in [-2\sigma, 2\sigma]$ are real valued quenched random variables with $\sigma \geq 0$ setting the strength of the disorder. The constraint $\sum_{l \text{ n.n. of } k} n_{(kl)} = 0$ means that at all lattice sites k the incoming flow has to balance the outgoing flow, i. e. the flow $\{n_{\mathbf{i}}\}$ is divergence-less. The physical motivation of studying models these kind of models is the following:

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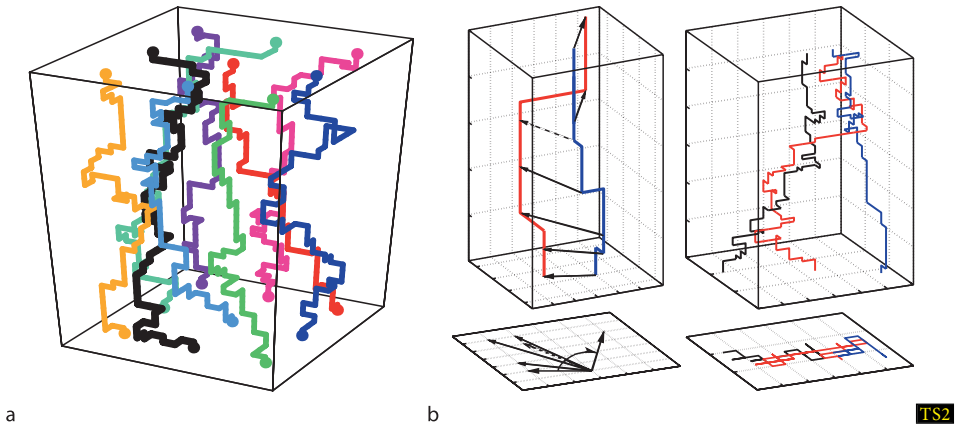
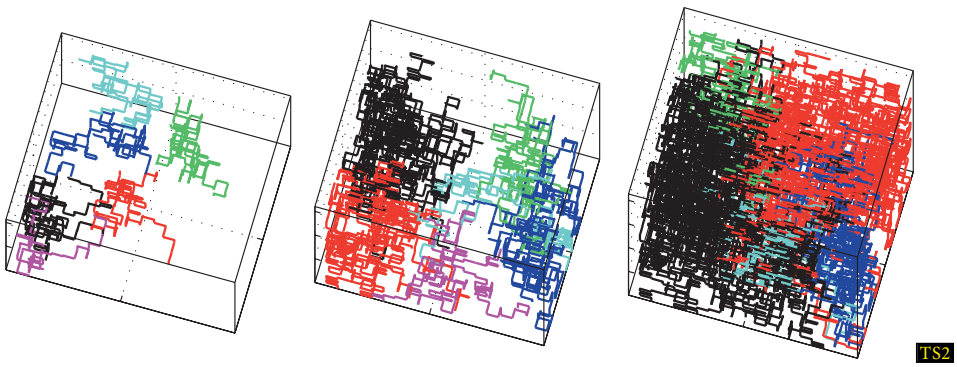


Optimization Problems and Algorithms from Computer Science, Figure 2
Left: **Ground state configuration of a *N*-line system with $N = 9$ defined by (8). The entry/exit points are fixed in a regular 3×3 array for better visibility.** ***Right:*** **Definition of the winding angle of two flux lines.** ***Right part, top*****: A configuration of three lines that are entangled.** ***Right part, bottom*****: The projection of the line configuration on the basal plane, defining a connected cluster**



Optimization Problems and Algorithms from Computer Science, Figure 3
Line configurations for different heights *H* (*from left to right*: $H = 64, 96, 128$), the lateral size $L = 20$, the line density is $\rho = 0.3$. Only the largest line bundles are shown, indicated by a varying gray scale. *Black* denotes the largest cluster, which eventually percolates

In 2d the Hamiltonian (9) occurs for instance in the context of the solid-on-solid (SOS) model on a disordered substrate [19]. The SOS representation of a 2d surface is defined by integer height variables u_k for each lattice site k of a square lattice. The disordered substrate is modeled via random offsets $d_k \in [0,1]$ for each lattice site, such that the total height at lattice site k is $h_k = u_k + d_k$. The the total energy of the surface is

$$\mathcal{H}_{\mathrm{SOS}} = \sum_{(kl)} (h_k - h_l)^2 = \sum_{(\tilde{kl})} \left(n_{(\tilde{kl})} - b_{(\tilde{kl})} \right)^2 \qquad (10)$$

where the first sum runs over all nearest neighbor pairs (kl) of the square lattice and the second sum runs over all bonds $(\tilde{kl})$ of the *dual* lattice (being a square lattice, too), which connect the centers of the elementary plaquettes of the original lattice. A dual bond $(\tilde{kl})$ therefore crosses perpendicularly a bond (kl) connecting neighbors k and l on the original lattice. We define $n_{(\tilde{kl})} = n_k - n_l$ and $d_{(\tilde{kl})} = d_l - d_k$ if l is either the right or the upper neighbor of k (i. e. for $k = (x, y)$ either $l = (x+1, y)$ or $l = (x, y+1)$ and $n_{(\tilde{kl})} = n_l - n_k$ and $d_{(\tilde{kl})} = d_k - d_l$ if l is either the left or the lower neighbor of k (i. e. for $k = (x, y)$ either $l = (x-1, y)$ or $l = (x, y-1)$. In this way the sum over all four dual bond variables attached to one site of the dual lattice corresponds to the sum of original height variables around an elementary plaquette in the original lattice: $(n_{(x,y)} - n_{(x,y+1)}) + (n_{(x,y+1)} - n_{(x+1,y+1)}) + (n_{(x+1,y+1)} - n_{(x+1,y)}) + (n_{(x+1,y)} - n_{(x,y)}) = 0$, which implies that the flow $\{n_{(\tilde{kl})}\}$ is divergence free as inferred in (9).

In 3d the Hamiltonian (9) is the strong screening limit of the vortex glass model for disordered superconduc-

tors [20,21]

$$\mathcal{H}_{\mathrm{VG}} = \sum_{i,j} (n_i - b_i) G_\lambda(\mathbf{r}_i - \mathbf{r}_j)(n_j - b_j)\,, \tag{11}$$

where the integer vortex variables n_i live on the bonds of a simple cubic lattice and have to fulfill the constraint in (9) since they represent magnetic vortex lines that are divergence free. The real valued quenched random variables $b_i \in [-2\sigma, 2\sigma]$ are derived from the lattice curl of a random vector potential ($\sigma \geq 0$ being the strength of the disorder). The 3d vector $\mathbf{r}_i$ denotes the spatial positions of bond i in the lattice and the sum runs over all bond pairs of the lattice (not only nearest neighbors). The lattice propagator $G_\lambda(\mathbf{r})$ has the asymptotic form $G_\lambda(\mathbf{r}) \propto \exp(-|\mathbf{r}|/\lambda)/|\mathbf{r}|$, where λ is the screening length. In the strong screening limit $\lambda \to 0$ only the on-site repulsion survives [20] and gets

$$\mathcal{H}_{\mathrm{VG}}^{\lambda\to 0} = \sum_i (n_i - b_i)^2 \tag{12}$$

which is the Hamiltonian (9) in 3d that we intend to discuss here.

The ground state of (9) can again be computed within polynomial time by a successive shortest path algorithm [3]. As for the N-line problem one starts with a configuration $\{n_{\mathbf{i}}\}$ that optimizes the Hamiltonian in (9) but does not, in general, fulfill the mass balance constraint given in (9). In the N-line problem that was simply the zero-flow $n_{\mathbf{i}} = 0$, which does not fulfill the requirement that the source and the target have excess $+N$ and $-N$, respectively. Here we start with $n_{\mathbf{i}}$ the closest integer to the real number $b_{\mathbf{i}}$ for each bond $\mathbf{i}$. Since this solution violates the mass-balance constraint one successively sends flow from nodes that have an excess flow to nodes that have a deficit along optimal paths that are again found using node potentials (to make all costs non-negative) and Dijkstra's algorithm. The details of this algorithm can be found in [1,2,3].

Figure 4 shows three typical ground state configurations for different strength of the disorder σ in 2d and in 3d. For small σ only small isolated loops occur, whereas for larger σ one finds loops that extend through the whole system, they percolate. A finite size scaling study of the underlying percolation transition [22] yields a novel universality class with numerically estimated critical exponents that differ significantly from those for conventional bond- or site-percolation [22].

Interfaces and Elastic Manifolds

A system of strongly interacting (classical) particles or other objects, like magnetic flux lines in a type-II superconductor (as we discussed in Sect. "Many Repulsive Elastic Lines in Random Media" and for which the starting Hamiltonian would given by (7)), or a charge density wave system in a solid, will order at low temperatures into a regular arrangement a lattice (crystal lattice or flux line lattice). Fluctuations either induced by thermal noise (temperature) or by disorder (impurities, pinning centers) induce deviations of the individual particles from their equilibrium positions. As long as these fluctuations are not too strong an expansion of the potential energy around these equilibrium configuration might be appropriate. An expansion up to 2nd order is called the elastic description or elastic approximation, which in a coarse grained form (where the individual particles that undergo displacements from their equilibrium positions do not occur any more and are replaced by a continuum field $\phi(\mathbf{r})$ reads then

$$\begin{aligned}\mathcal{H}_{\mathrm{manifold}} &= \mathcal{H}_{\mathrm{elastic}} + \mathcal{H}_{\mathrm{random}} \\ &= \int \mathrm{d}^d\mathbf{r} \left\{ \frac{\gamma}{2} |\nabla\phi(\mathbf{r})|^2 + V(\phi(\mathbf{r}), \mathbf{r}) \right\}\,.\end{aligned} \tag{13}$$

The random potential energy is a delta-correlated Gaussian variable with mean zero, $\langle\langle V(\phi,\mathbf{r}) V(\phi',\mathbf{r}')\rangle\rangle = D^2\delta(\phi-\phi')\delta(\mathbf{r}-\mathbf{r}')$. The integration extends over the whole space that parameterizes the manifold, for instance $d = 1$ for an elastic line in a random potential, $d = 2$ for an interface or a surface in a disordered environment etc. Note that for $d = 1$ one recovers the single line Hamiltonian (3). The many-line Hamiltonian (7) also allows such an elastic description in the limit, in which the interactions are strong and the the random potential is weak compared to the elastic energy. In this limit the lines will only deviate moderately from a regular, translationally invariant configuration (the Abrikosov flux line lattice). This case is called an elastic periodic medium and one has to modify the φ-part of the disorder correlator such that the Hamiltonian has the correct translational symmetry [26].

Elastic Manifold

The typical example for an elastic manifold in a disordered environment are domain walls in the $d+1$ dimensional random bond ferromagnet $H = -\sum_{\langle ij\rangle} J_{ij}\sigma_i\sigma_j$ ($J_{ij} \geq 0$, random) in which we fix all spins in the lower (upper) plane, i. e. all σ_i with $i = (x_1 1, \ldots, x_d, y)$ and $y = 1$ ($y = H$), to be $\sigma_i = +1(-1)$, c.f. Fig. 5. First one maps it onto a flow problem in a capacitated network. One introduces two extra sites, a source node s, which is connected to all spins of the hyperplane $y = 1$ with bonds $J_{s,(x_1,\ldots,x_d,y=1)} = J_\infty$, and a sink node t, which is connected to all spins of the hyperplane $y = H$ with bonds $J_{s,(x_1,\ldots,x_d,y=H)} = J_\infty$. One chooses $J_\infty = 2\sum_{(ij)} J_{ij}$, i. e. strong enough that the interface cannot pass through a bond involving one of

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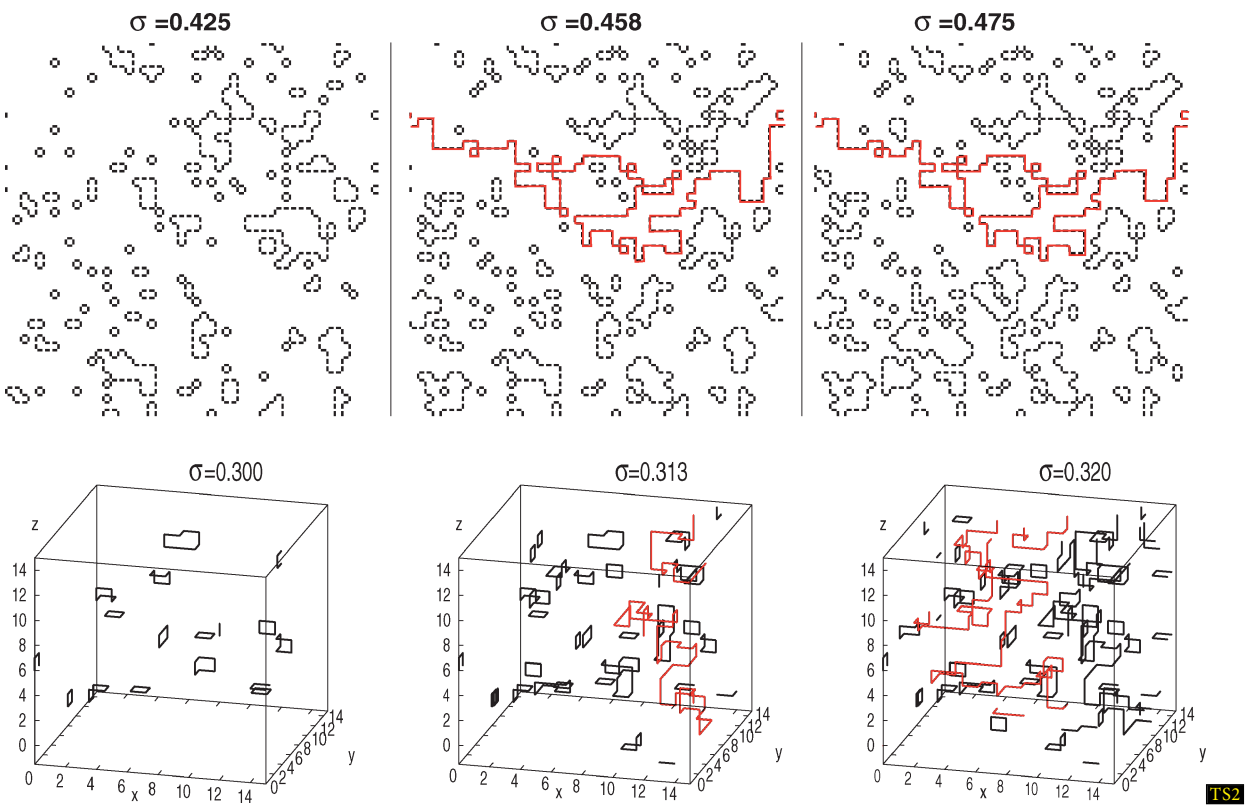


Optimization Problems and Algorithms from Computer Science, Figure 4
Examples of ground state configurations of the Hamiltonian (9) for varying disorder strengths σ (for particular disorder realizations). *Top*: 2d, $L = 50$, the critical disorder strength is $\sigma_c \approx 0.46$; *Bottom*: 3d, $L = 16$, the critical disorder strength is $\sigma_c \approx 0.31$. The occupied bonds ($n_i \neq 0$) are marked *black*, the percolating loop is marked by *light gray (red)* TS3

the two extra sites. Now we enforce the aforementioned boundary conditions for the spins in the upper and the lower plane by simply fixing $\sigma_s = +1$ and $\sigma_t = -1$. The graph underlying the capacitated network one has to consider is now defined by the set of vertices (or nodes) $N = \{1, \ldots, H \cdot L^d\} \cup \{s, t\}$ and the set of edges (or arcs) connecting them $A = \{(i, j) | i, j \in N,\ J_{ij} > 0\}$.

The capacities $u_i j$ of the arcs (i, j) is given by the bond strength $J_i j$. For any spin configuration $\sigma = (\sigma_1, \ldots, \sigma_N)$ one defines $S = \{i \in N | \sigma_i = +1\}$ and $\overline{S} = \{i \in N | \sigma_i = -1\} = N \backslash S$. Obviously $\sigma_s \in S$ and $\sigma_t \in \overline{S}$. The knowledge of S is sufficient to determine the energy of any spin configuration via $H(S) = -C + 2 \sum_{(i,j) \in (S,\overline{S})} J_{ij}$ where $(S, \overline{S}) = \{(i, j) | i \in S, j \in \overline{S}\}$. The constant $C = \sum_{(i,j) \in A} J_{ij}$ is irrelevant, i. e. independent of S. Note that $(S, \overline{S})$ is the set of edges (or arcs) connecting S with $\overline{S}$, this means it cuts N in two disjoint sets. Since $s \in S$ and $t \in \overline{S}$, this is a so called s-t-cut-set, abbreviated $[S, \overline{S}]$. Thus the problem of finding the ground state configuration of an interface in the random bond ferromagnet can be reformulated as a **minimum cut** problem

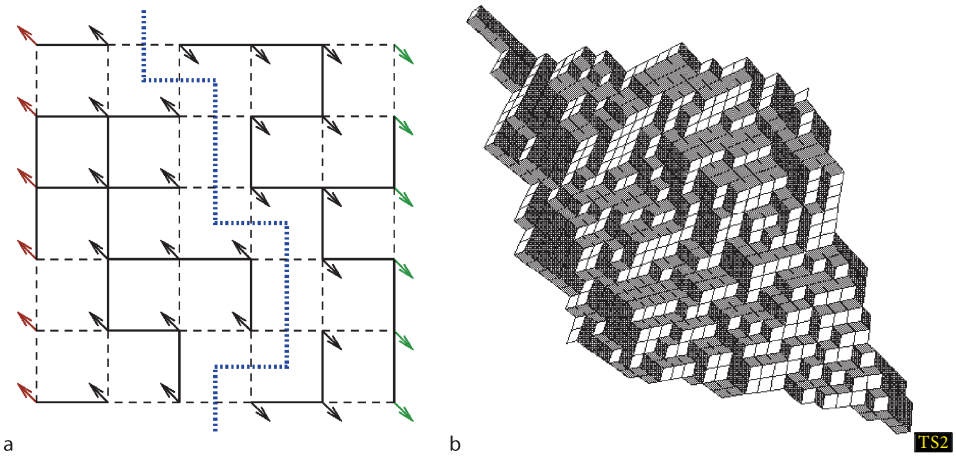
$$\min_{S \subset N} \{H'(S)\} = \min_{[S,\overline{S}]} \sum_{(i,j) \in (S,\overline{S})} J_{ij} \,. \tag{14}$$

in the above defined capacitated network (with $H' = (H + C)/2$). It does not come as a surprise that this minimum cut is *identical* with the interface between the $(\sigma_i = +1)$-domain and the $(\sigma_i = -1)$-domain that has the lowest energy. Actually any s-t-cut-set defines such an interface, some of them might consist of many components, which is of course energetically unfavorable.

A flow in the network G is a set of nonnegative numbers x_{ij} subject to a capacity constraint and a mass balance constraint for each arc

$$0 \leq x_{ij} \leq u_{ij}$$

$$\text{and} \quad \sum_{\{j|(i,j) \in A\}} x_{ij} - \sum_{\{j|(j,i) \in A\}} x_{ji} = \begin{cases} -v & \text{for } i = s \\ +v & \text{for } i = t \\ 0 & \text{else} \end{cases} \tag{15}$$



Optimization Problems and Algorithms from Computer Science, Figure 5
Left: **Sketch of a 2d (RBIM) with antiperiodic boundary conditions.** ***Broken lines*** **represent weak bonds,** ***full lines*** **strong bonds, the spin configuration with the lowest energy defines an interface, as indicated, and corresponds to the minimum cut in the corresponding network flow problem.** ***Right:*** **An optimal interface in the 111-direction of a 3d RBIM corresponding to the ground state configuration of a 2d elastic medium with scalar displacement field (from [23])**

This means that at each node everything that goes in has to go out, too, with the only exception being the source and the sink. What actually flows from s to t is v, the value of the flow. The **maximum flow problem** for the capacitated network G is simply to find the flow $\mathbf{x}$ that has the maximum value v under the constraint (15).

Let $\mathbf{x}$ be a flow, v its value and $[S, \overline{S}]$ an s-t-cut. Then, by adding the mass balances for all nodes in S one has $v = \sum_{(i,j)\in(S,\overline{S})} x_{ij} - \sum_{(i,j)\in(\overline{S},S)} x_{ji}$ and since $x_{ij} \leq u_{ij}$ and $x_{ji} \geq 0$ the following inequality holds: $v \leq \sum_{(i,j)\in(S,\overline{S})} u_{ij} = u[S, \overline{S}]$. Thus the value of any flow $\mathbf{x}$ is less or equal to the capacity of any cut in the network. If one discovers a flow $\mathbf{x}$ whose value equals to the capacity of some cut $[S, \overline{S}]$, then $\mathbf{x}$ is a maximum flow and the cut is a minimum cut. The following implementation of the augmenting path algorithm constructs a flow whose value is equal to the capacity of a s-t-cut it defines simultaneously. Thus it will solve the maximum flow problem (and, of course, the minimum cut problem).

Given a flow $\mathbf{x}$, the residual capacity $r_i j$ of any arc $(i, j) \in A$ is the maximum additional flow that can be sent from node i to node j using the arcs (i,j) and (j, i). The residual capacity has two components: 1) $u_{ij} - x_{ij}$, the unused capacity of arc (i,j), 2) $x_j i$ the current flow on arc (j, i), which one can cancel to increase the flow from node i to j $r_{ij} = u_{ij} - x_{ij} + x_{ji}$. The residual network $G(\mathbf{x})$ with respect to the flow $\mathbf{x}$ consists of the arcs with *positive* residual capacities. An augmenting path is a directed path from the node s to the node t in the residual network. The *capacity of an augmenting path* is the minimum residual capacity of any arc in this path.

Obviously, whenever there is an augmenting path in the residual network $G(\mathbf{x})$ the flow $\mathbf{x}$ is not optimal. This motivates the following generic augmenting path algorithm:

algorithm Ford–Fulkerson
begin
  Initially set $x_{ij} := 0, x_{ji} := 0$ for all $(i, j) \in A$;
  do
    construct residual network R with capacities r_{ij};
    if there is an augmenting path from s to t in G' **then**
    begin
      Let $r_{\min}$ the minimum capacity of r along this path;
      Increase the flow in N along the path
        by a value of $r_{\min}$;
    end
  until no such path from s to t in G' is found;
end CE4

This algorithm is polynomial in the number of lattice sites if the distribution of capacities is discrete (binary for instance). In the general case it has to be improved and there are indeed more efficient algorithms to solve this problem in polynomial time. One of them is the push/relabel algorithm introduced by Goldberg and Tarjan [24]. It determines the maximal flow by successively improving a "preflow". A preflow is an edge function $f(e)$ that obeys the range constraint $0 \leq f(e) \leq w(e)$, but the conservation constraint at each node is relaxed: the sum of the $f(e)$ into or out of a node can be nonzero at internal (physical) nodes. The amount of violation of conservation at each node v give "excesses" $e(v)$. The basic operations of the algorithm, push and relabel, are used to rearrange these

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excesses. When the preflow can no longer be improved, it can, if desired, be converted to a maximal flow, proving the correctness of the algorithm. For details see [24,25]. It can be applied in the way sketched above to compute universal geometrical properties of elastic manifolds in 2 and 3 dimensions [23].

Periodic Medium

The presence of a periodic background potential, like a crystal potential, has a smoothening effect on the elastic manifold and tends to lock it into one of its minima. The competition between the random potential, that roughens the manifold, and such a periodic potential might lead to a roughening transition [27,28]. In 2d this is actually not the case [29], but in 3d there is as we will see. We consider a lattice version of the Hamiltonian

$$\begin{aligned} &\mathcal{H} = \mathcal{H}_{\text{manifold}} + H_{\text{periodic}} \\ &\text{with} \quad H_{\text{periodic}} = \int \mathrm{d}^d\mathbf{r}\; V_{\text{periodic}}(\phi(\mathbf{r}))\,, \end{aligned} \tag{16}$$

where $V_{\text{periodic}}(\phi) = -\cos\phi$ represents the periodic potential.

We introduce a discrete solid-on-solid (SOS) type interface model for the elastic manifold whose continuum Hamiltonian is given in Eq. (16). Locally the EM remains flat in one of periodic potential minima at $\phi = 2\pi h$ with integer h. Due to fluctuations, some regions might shift to a different minimum with another value of h to create a step (or domain wall) separating domains. To minimize the cost of the elastic and periodic potential energy in Eq. (16), the domain-wall width must be finite, say ξ_o. Therefore, if one neglects fluctuations in length scales less than ξ_o, the continuous displacement field $\phi(\mathbf{r})$ can be replaced by the integer height variable $\{h_{\mathbf{x}}\}$ representing a $(3+1)d$ SOS interface on a simple cubic lattice with sites $\mathbf{x} \in \{1,\ldots,L\}^3$. The lattice constant is of order ξ_o and set to unity. The energy of the interface is given by the Hamiltonian

$$\mathcal{H} = \sum_{\langle \mathbf{x},\mathbf{y}\rangle} J_{(h_{\mathbf{x}},\mathbf{x});(h_{\mathbf{y}},\mathbf{y})} |h_{\mathbf{x}} - h_{\mathbf{y}}| - \sum_{\mathbf{x}} V_R(h_{\mathbf{x}},\mathbf{x})\,, \tag{17}$$

where the first sum is over nearest neighbor site pairs. After the coarse graining, the step energy $J > 0$ as well as the random pinning potential energy V_R becomes a quenched random variable distributed independently and randomly. Note a periodic elastic medium has the same Hamiltonian as in Eq. (17) with random but periodic J and V_R in h with periodicity p [30]. In this sense, the elastic manifold emerges as in the limit $p \to \infty$ of the periodic elastic medium.

To find the ground state, one maps the 3D SOS model onto a ferromagnetic random bond Ising model in $(3+1)$d hyper-cubic lattice with anti-periodic boundary conditions in the extra dimension [23] (for the 3 space direction one uses periodic boundary conditions instead). The anti-periodic boundary conditions force a domain wall into the ground state configuration of the $(3+1)$d ferromagnet. Note that bubbles are *not* present in the ground state. A domain wall may contain an overhang which is unphysical in the interface interpretation. Fortunately, one can forbid overhangs in the Ising model representation using a technique described in [23]. If the longitudinal and transversal bond strengths are assigned with $J/2$ and $V_R/2$ occurring in Eq. (17), respectively, this domain wall of the ferromagnet becomes equivalent to the ground state configuration of (17) for the interface with the same energy. The domain wall with the lowest energy is then determined exactly by using again the max-flow/min-cost algorithm.

In elastic media described by (17) the tendency of the periodic potential to lock the displacements competes with the roughening effect of the disorder. Analytically a roughening transition was predicted in [28] and the critical exponents could be numerically estimated in three dimensions [30] with the mapping and algorithm described above.

Random Field Ising Model

The random field Ising model (RFIM, for a review see [31, 32]) is defined

$$H = -\sum_{(ij)} J_{ij}\sigma_i\sigma_j - \sum_i h_i\sigma_i \tag{18}$$

with $\sigma_i = \pm 1$ Ising spins, ferromagnetic bonds $J_{ij} \geq 0$ (random or uniform), (ij) nearest neighbor pairs on a d-dimensional lattice and at each site i a random field $h_i \in R$ that can be positive and negative. The first term prefers a ferromagnetic order, which means it tries to align all spins. The random field, however, tends to align the spins with the field which points in random directions depending on whether it is positive or negative. This is the source of competition in this model.

Let us suppose for the moment uniform interactions $J_{ij} = J$ and a symmetric distribution of the random fields with mean zero and variance h_r. It is established by now that in 3d (and higher dimensions) the RFIM shows ferromagnetic long range order at low temperatures, provided h_r is small enough. In 1d and 2d there is no ordered phase at any finite temperature. Thus in 3d one has a para-

magnetic/ferromagnetic phase transition along a line $h_c(T)$ in the h_r-T-diagram.

The renormalization group picture says that the nature of the transition is the same all along the line $h_c(T)$, with the exception being the pure fixed point at $h_r = 0$ and $T_c \sim 4.51\,J$. The RG flow is dominated by a zero temperature fixed point at $h_c(T = 0)$. As a consequence, the critical exponents determining the critical behavior of the RFIM should be all identical along the phase transition line, in particular identical to those one obtains *at zero temperature* by varying h_r alone. Thus to study the universal properties of the phase transition in the RFIM one needs to calculate its ground state.

This optimization task is again equivalent to a maximum flow problem [33,34], as in the interface model discussed in the last section. Historically the RFIM was the first physical model that has been investigated with a maximum flow algorithm [36]. However, here the minimum-cut is not a geometric object within the original system.

To map the ground state problem for the RFIM onto a max-flow-min-cut problem one proceeds in the same way as in the interface problem: One adds to extra nodes s and t and attaches spins with fixed values there (see Fig. 6):

$$\sigma_s = +1 \qquad \text{and} \qquad \sigma_t = -1 \tag{19}$$

One connects all sites with positive random field to the node s and all sites with negative random field to t:

$$\begin{aligned} J_{si} &= \begin{cases} h_i & \text{if } h_i \geq 0 \\ 0 & \text{if } h_i < 0 \end{cases} \\ J_{it} &= \begin{cases} |h_i| & \text{if } h_i < 0 \\ 0 & \text{if } h_i \geq 0 \end{cases} \end{aligned} \tag{20}$$

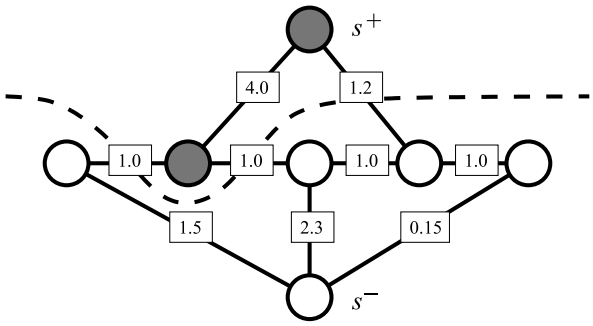
The a network is constructed with the set of nodes $N = \{1, \cdots, L^d\} \cup \{s, t\}$ and the set of (forward and backward) arcs $A = \{(i, j) | i, j \in N,\ J_{ij} > 0\}$. Each of them has a capacity $u_{ij} = J_{ij}$. The energy or cost function can the be written as

$$E = -\sum_{(i,j)\in A} J_{ij}\sigma_i\sigma_j \tag{21}$$

or, by denoting the set $S = \{i \in N | S_i = +1\}$ and $\overline{S} = N \backslash S$

$$E(S) = -C + 2 \sum_{(i,j)\in(S,\overline{S})} J_{ij} \tag{22}$$

with $C = \sum_{(i,j)\in A} J_{ij}$. The problem is reduced to the problem of finding a minimum s-t-cut as in (14). The difference to the interface problem is that now the extra bonds connecting the two special nodes s and t with the original lattice do not have infinite capacity: they can lie *in* the cut,



Optimization Problems and Algorithms from Computer Science, Figure 6

Representation of the ground state problem for the RFIM as an RBIM domain wall or minimum-cut problem. The physical spins are the five nodes in the single row in the figure, while the fixed external spins are s^+ and s^-. The physical RFIM coupling $J = 1.0$. A spin with $h_i > 0$ ($h_i < 0$) is connected by an auxiliary coupling of strength h_i ($-h_i$) to s^+ (s^-). The weights of each bond are indicated: the random fields are, *from left to right*, $h = -1.5, +4.0, -2.3, +1.2$, and 0.15. In the ground state, the interfacial energy between up-spin and down-spin domains is minimized, i. e., the spins are partitioned into two sets with minimal total cost for the bonds connecting the two sets. The *dashed* curve indicates the minimal weight cut. The *white (dark)* nodes indicate up (down) spins in the ground state configuration

namely whenever it is more favorable not to break a ferromagnetic bond but to disalign a spin with its local random field. In the extended graph the s-t-cut again forms connected interface, however, in the original lattice (without the bonds leading to and from the extra nodes) the resulting structure is generally *disconnected*, a multicomponent interface. Each single component surrounds a connected region in the original lattice containing spins, which all point in the same direction. In other words, they form ferromagnetically ordered domains separated by domain walls given by the subset of the s-t-cut that lies in the original lattice.

In passing we note that diluted Ising antiferromagnets in a homogeneous external field (DAFF) map straightforwardly onto a RFIM if the underlying lattice is bipartite. The 3d DAFF on a simple cubic lattice is defined by

$$H = +\sum_{(ij)} J_{ij}\varepsilon_i\varepsilon_j\sigma_i\sigma_j - \sum_i h_i\varepsilon_i\sigma_i \tag{23}$$

where $\sigma_i = \pm 1$, $J_{ij} \geq 0$, (ij) are nearest neighbor pairs on a simple cubic lattice, and $\varepsilon_i \in \{0, 1\}$ with $\varepsilon_i = 1$ with probability c, representing the concentration of spins. Because of the plus sign in front of the first term in (23) all interactions are antiferromagnetic, the model represents a diluted antiferromagnet, for which many experimental realizations exist (e. g. $Fe_cZn_{1-c}F_2$). Now that neighboring spins tend

to point in opposite directions due to their antiferromagnetic interaction a uniform field competes with this ordering tendency by trying to align them all. On a bipartite lattice in zero external field the ground state would be antiferromagnetic, which means that one can define two bipartite sublattices A and B. One defines new spin and field variables via

$$\sigma_i' = \begin{cases} +\sigma_i & \text{for } i \in A \\ -\sigma_i & \text{for } i \in B \end{cases}$$
$$h_i' = \begin{cases} +\varepsilon_i h_i & \text{for } i \in A \\ -\varepsilon_i h_i & \text{for } i \in B \end{cases} .$$

Since $\sigma_i'\sigma_j' = -\sigma_i\sigma_j$ for all nearest neighbor pairs (ij) one can write (23) as

$$H = -\sum_{(ij)} J_{ij}'\sigma_i'\sigma_j' - \sum_i h_i'\sigma_i' \tag{24}$$

with $J_{ij}' = J_{ij}\varepsilon_i\varepsilon_j$. This is again a RFIM and ground states can be computed with the max-flow technique.

The main focus of the application of the max-flow-min-cut algorithm to the RFIM is the phase transition in the three-dimensional model occurring at a critical disorder strength h_c at zero temperature, which separates a paramagnetic phase for large disorder strength from a ferromagnetic phase. The maximum flow algorithm has first been used by Ogielski [36] to calculate the critical exponents of the RFIM via the finite size scaling. More accurate estimates were obtained more recently by Middleton and Fisher [35], where also an detailed discussion of the problems and conflicting results about the RFIM universality class is provided. For Gaussian random fields (with variance h^2) they find for the finite size scaling of magnetization $m = [S_i]\text{av}$ and specific heat $c = N^{-1}\mathrm{d}E/\mathrm{d}T$ and

$$\begin{aligned} m &\sim L^{-\beta/\nu} , \\ c &\sim L^{\alpha/\nu} , \end{aligned} \tag{25}$$

with the magnetization exponent $x = \beta/\nu = 0.012 \pm 0.004$ the correlation length exponent $\nu = 1.37 \pm 0.09$, and the specific heat exponent $\alpha = -0.07 \pm 0.17$. Note that the magnetization exponent is very close to zero, which means that the transition is hard to discriminate from a first order transition. Also the specific heat exponents is close to zero and slightly negative, implying a lack of divergence of the specific heat at the transition.

The Spin Glass Problem

Spin glasses are the prototypes of (disordered) frustrated systems (see [37]). In the models discussed up to now, the frustration was caused by two separate terms of different physical origin (interactions and external fields or boundary conditions). Spin glasses are magnetic systems in which the magnetic moments interact ferro- or antiferromagnetically in a random way, as in the following Edwards–Anderson Hamiltonian for a short ranged Ising spin glass (SG)

$$H = -\sum_{(ij)} J_{ij}\sigma_i\sigma_j , \tag{26}$$

where $\sigma_i = \pm 1$, (ij) are nearest neighbor interactions on a d-dimensional lattice and the interaction strengths $J_{ij} \in R$ are unrestricted in sign. In analogy to Eq. (14) one shows that the problem of finding the ground state is again equivalent to finding a minimal cut $[S, \bar{S}]$ in a network

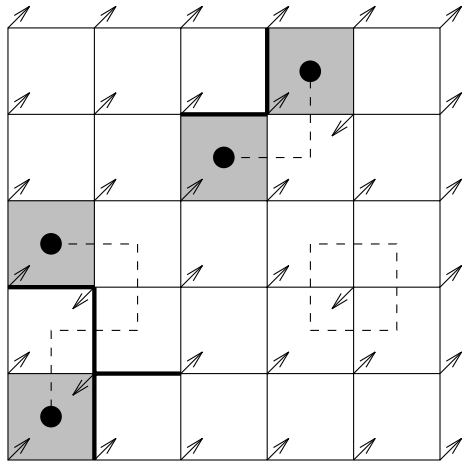
$$\min_{\underline{\sigma}} \{H'(\underline{\sigma})\} = \min_{[S,\bar{S}]} \sum_{(i,j)\in(S,\bar{S})} J_{ij} , \tag{27}$$

again $H' = (H + C)/2$ with $C = \sum_{(ij)} J_{ij}$. However, now the capacities $u_{ij} = J_{ij}$ of the underlying network are *not* non-negative any more, therefore it is *not* a minimum-cut problem and thus it is also not equivalent to a maximum flow problem, which we know how to handle efficiently.

It turns out that the spin glass problem is *much* harder than the questions we have discussed so far. In general (i. e. in any dimension larger than two and also for 2d in the presence of an external field) the problem of finding the SG ground state is $\mathcal{NP}$-complete [42], which means in essence that no polynomial algorithm for it is known (and also that chances to find one in the future are marginal). Nevertheless, some extremely efficient algorithms for it have been developed [38,39], which have a non-polynomial bound for their worst case running-time but which terminate (i. e. find the optimal solution) after a reasonable computing time for pretty respectable system sizes.

Two Dimensions, Planar Graph

First we discuss the only non-trivial case that can be solved with a polynomial algorithm: the two-dimensional Ising SG on a planar graph. This problem can be shown to be equivalent to finding a minimum weight perfect matching, which can be solved in polynomial time. We do not treat matching problems and the algorithms to solve them in this lecture (see [4,40,41]), however, we would like to present the idea [42]. To be concrete let us consider a square lattice with free boundary conditions. Given a spin configuration $\underline{\sigma}$ (which is equivalent to $-\underline{\sigma}$) we say that an edge (or arc) (i,j) is satisfied if $J_{ij}\sigma_i\sigma_j > 0$ and it is *unsatisfied* if $J_{ij}\sigma_i\sigma_j < 0$. Furthermore we say a plaquette (i. e. a unit cell of the square lattice) is *frustrated* if it is surrounded by



Optimization Problems and Algorithms from Computer Science, Figure 7
Two-dimensional Ising spin glass with ±-J couplings: *Thin* lines, are positive interactions, *thick* lines are negative interactions, ↗ means $\sigma_i = +1$, ↙ means $\sigma_i = -1$, *shaded* faces are frustrated plaquettes, *broken* lines cross unsatisfied edges

an odd number of negative bonds (i. e. $J_{ij} \cdot J_{jk} \cdot J_{kl} \cdot J_{li} < 0$ with i, j, k and l the four corners of the plaquette)). There is a one-to-one correspondence between equivalent spin configurations ($\underline{\sigma}$ and $-\underline{\sigma}$) and sets of unsatisfied edges with the property that on each frustrated (unfrustrated) plaquette there is an odd (even) number of unsatisfied edges. See Fig. 7 for illustration.

Note that

$$H(\underline{\sigma}) = -C + 2 \sum_{\text{unsatisfied edges}} |J_{ij}| \,. \tag{28}$$

which means that one has to minimize the sum over the weights of unsatisfied edges. A set of unsatisfied edges will be constituted by a set of paths (in the dual lattice) from one frustrated plaquette to another and a set of closed circles (see Fig. 7). Obviously the latter always increase the energy so that we can neglect them. The problem of finding the ground state is therefore equivalent to finding the minimum possible sum of the weights of these paths between the frustrated plaquettes. This means that we have to *match* the black dots in the Fig. 7 with one another in an optimal way. One can map this problem on a minimum weight **perfect matching** problem (a perfect matching of a graph $G = (N, A)$ is a set $M \subseteq A$ such that each node has only has only one edge of M adjacent to it). This can be solved in polynomial time (see [42] for further details).

Note that for binary couplings, i. e. $J_{ij} = \pm J$, where $J_{ij} = +J$ with probability p the weight of a matching is simply proportional to the sum of the lengths of the various paths connecting the centers of the frustrated plaquettes, which simplifies the actual implementation of the algorithm. In [43] the 2d $\pm J$ spin glass and the site disordered SG has been studied extensively with this algorithm. The site disordered spin glass is defined as follows: occupy the sites of a square lattice randomly with A (with concentration c) and B (with concentration $1 - c$) atoms. Now define the interactions J_{ij} between neighboring atoms: $J_{ij} = -J$ if on both sites are A-atoms and J_{ij} otherwise.

The main application of this algorithm is directed towards studying domain walls in spin glasses since they provide informations on the low temperature behavior and the stability of the ground state with respect to thermal fluctuations. Domain walls can be induced by applying two different boundary conditions to the system (usually periodic and anti-periodic), their energy is simply the difference between the energies of the ground states with the two different boundary conditions. The domain wall energy of the two-dimensional spin glass model with Gaussian couplings scales like

$$\Delta E \sim L^{\theta} \,, \tag{29}$$

where the stiffness exponent is $\theta = -0.282$ (see [44] for a survey). The negativity of this exponent indicates the absence of stable spin glass phase at any non-vanishing temperature in the 2d spin glass model. Recently also the fractal properties of the domain walls in 2d spin glasses with Gaussian couplings became important: They have a fractal dimension of $d_f = 1.27(1)$ and it was argued [45] that they might be a realization of a stochastic Loewner evolution (see [46] for a review) realized in disordered systems.

Three Dimensions, Non-planar Graphs

As we mentioned, in any other case except the planar lattice situation discussed above the spin glass problem is $\mathcal{NP}$-hard. In what follows we would like to sketch the idea of an efficient but non-polynomial algorithm [39]. To avoid confusion with the minimum cut problem we discussed in connection with maximum flows one calls the problem (27) a max-cut problem (since finding the minimum of H is equivalent to finding the maximum of $-H$).

Let us consider the vector space R^A. For each cut $[S, \overline{S}]$ define $\chi^{(S,\overline{S})} \in R^A$, the incidence vector of the cut, by $\chi_e^{(S,\overline{S})} = 1$ for each edge $e = (i, j) \in (S, \overline{S})$ and $\chi_e^{(S,\overline{S})} = 0$ otherwise. Thus there is a one-to-one correspondence between cuts in G and their $\{0,1\}$-incidence vectors in R^A. The *cut-polytope* $P_C(G)$ of G is the convex hull of all incidence vectors of cuts in G: $P_C(G) = \text{conv}\,\{\chi^{(S,\overline{S})} \in R^A \mid S \subseteq A\}$. Then the max-cut problem can be written as a *linear pro-*

gram

$$\max \{\underline{u}^T \underline{x} \mid \underline{x} \in P_C(G)\} \tag{30}$$

since the vertices of $P_C(G)$ are cuts of G and vice versa. Linear programs usually consist of a linear cost function $\underline{u}^T \underline{x}$ that has to be maximized under the constraint of various inequalities defining a polytope in R^n (i. e. the convex hull of finite subsets of R^n) and can be solved for example by the simplex method, which proceeds from corner to corner of that polytope to find the maximum (see e. g. [40,41,48]). The crucial problem in the present case is that it is $\mathcal{NP}$-hard to write down all inequalities that represent the cut polytope $P_C(G)$.

It turns out that also *partial* systems are useful, and this is the essential idea for an efficient algorithm to solve the general spin glass problem as well as the traveling salesman problem or other so called mixed integer problems (i. e. linear programs where some of the variables x are only allowed to take on some integer values, like 0 and 1 in our case) [7,47]. One chooses a system of linear inequalities L whose solution set $P(L)$ contains $P_C(G)$ and for which $P_C(G) = \text{convex hull } \{\mathbf{x} \in P(L) | x \text{ integer}\}$. In the present case these are $0 \le x \le 1$, which is trivial, and the so called cycle inequalities, which are based on the observation that all cycles in G have to intersect a cut an even number of times. The most remarkable feature of this set L of inequalities is the following:

The separation problem for a set of inequalities L consists in either proving that a vector x satisfies all inequalities of this class or to find an inequality that is violated by $\mathbf{x}$. A linear program can be solved in polynomial time if and only if the separation problem is solvable in polynomial time [49]. The separation problem for the cycle inequalities can be solved in polynomial time by the *cutting plane algorithm* which, starting from some small initial set of inequalities, generates iteratively new inequalities until the optimal solution for the actual subset of inequalities is feasible. Note that one does not solve this linear program by the simplex method since the cycle inequalities are still too numerous for this to work efficiently.

Due to the insufficient knowledge of the inequalities that are necessary to describe $P_C(G)$ completely, one may end up with a non-integral solution $\mathbf{x}^*$. In this case one *branches* on some fractional variable x_e (i. e. a variable with $x_e^* \notin \{0,1\}$), creating two subproblems in one of which x_e is set to 0 and in the other x_e is set to 1. Then one applies the cutting plane algorithm recursively for both subproblems, which is the origin of the name *branch-and-cut*. Note that in principle this algorithm is not restricted to any dimension, boundary conditions, or to the fieldless case. However, there are realizations of it that run fast (e. g. in 2d) and others that run slow (e. g. in 3d) and it is ongoing research to improve on the latter, for an overview over the current status see [47].

Potts Free Energy and Submodular Functions

The problem addressed in this chapter is not a low temperature problem but concerns the computation of the free energy of a Potts model (see [50] for a review) at *any temperature*, including some phase transition temperatures. To transform the problem of computing the free energy into an optimization problem (i. e. find a minimum in a finite set), one needs to take some limit. Usually this is a zero temperature limit as it was for all applications discussed so far in this article. Here this will be the limit of an *infinite number of states*.

Consider the q-state Potts model on a d-dimensional hyper-cubic lattice with periodic boundary conditions defined by the Hamiltonian:

$$H = -\sum_{\langle ij \rangle} J_{ij} \delta(\sigma_i, \sigma_j) \,, \tag{31}$$

where σ_i are q-state Potts variables ($\sigma_i \in \{1, \ldots, q\}$ located at lattice sites i, the sum goes over all nearest neighbor pairs $\langle ij \rangle$ of the lattice, and $J_{ij} > 0$ are ferromagnetic couplings (not that $\delta(\sigma, \sigma')$ is the Kronecker-delta, which means $\delta(\sigma, \sigma') = 1$ for $\sigma = \sigma'$ and $\delta(\sigma, \sigma') = 0$ for $\sigma \neq \sigma'$). The case $q = 2$ corresponds to the Ising model. In the random bond Potts model, which is of interest here, the couplings J_{ij} are random variables. In $d \le 2$ dimensions the Potts model has phase transition at some critical temperature T from a paramagnetic to a ferromagnetic phase. Thermodynamic properties of the q-state Potts model are computed via its partition function

$$\mathcal{Z} = \sum_{\{\underline{\sigma}\}} \exp\left(\sum_{ij} -\beta J_{ij} \delta(\sigma_i, \sigma_j)\right) . \tag{32}$$

The first sum runs over all possible spin configuration, i. e. it involves q^N terms, where N is the number of spins in the system and $\beta = 1/T$ is the inverse temperature.

In the so-called random cluster representation [51] the partition sum can be written as a sum over all subsets $U \subseteq E$ of the set of edges (or bonds)

$$\begin{aligned} \mathcal{Z} &= \sum_{\{\sigma\}} \prod_{ij} \exp\left(-\beta J_{ij} \delta(\sigma_i, \sigma_j)\right) \\ &= \sum_{\{\sigma\}} \prod_{ij} \left(1 + v_{ij} \delta(\sigma_i, \sigma_j)\right) \end{aligned}$$

where $v_{ij} = \exp(\beta K_{ij}) - 1$. Note that the Kronecker-delta can only take on the values zero and one by which it is

possible to identify $\exp(J\delta) = 1 + \delta(\exp(J) - 1) = 1 + v\delta$. Again one can regard the lattice as a graph $G = (V, E)$, where the sites and the bonds of the lattice are the vertices V and the edges E of the graph. Then a careful book-keeping of the terms in the development of the above expression leads to:

$$Z = \sum_{G' \subseteq G} q^{c(G')} \prod_{e \in G'} v_e \,, \tag{33}$$

where G' denotes any subgraph of G, i. e. a graph, possibly not connected (but all vertices are kept), where some edges of G have been deleted (there are 2^m subgraphs where m is the number of edges of G). $c(G')$ is the number of connected components of the subgraph G'. For example for the empty subgraph $G' = \varnothing$ the number of connected components is the number of sites, while for $G' = G$ it is one. The product in (33) is over all the edges in G' with the convention that the product over an empty set is one. If the parameter β is small (i. e. high temperature) then the parameters v_{ij} are small and, summing in (33), only the subgraphs with few edges provides an approximation to the partition function: this is a high temperature development. Note also the way the parameter q appears in (33): it can be extended to non integer values, relating the Potts model to other problems (percolation, etc ...) [58].

Following [52] one can map the computation of the partition function Z of any ferromagnetic Potts model in the limit $q \to \infty$ onto an optimization problem by introducing another parametrization of the couplings with new variables w_e defined by

$$v_e = q^{w_e} \,.$$

Inserting this expression in (33) one gets $Z = \sum_{G' \subseteq G} q^{c(G') + \sum_{e \in G'} w_e}$, and defining $f(G) = c(G) + \sum_{e \in G} w_e$:

$$Z = \sum_{G' \subseteq G} q^{f(G')} \,.$$

In the limit $q \to \infty$ only the subgraphs $G^\star$ maximizing $f(G)$ will contribute, and computing the partition function of the Potts model in the infinite number of states limit amounts to finding the subgraphs G' of the graph G maximizing the function f, i. e. minimizing the function [52]:

$$f_P(G') = -\left(c(G') + \sum_{e \in G'} w_e \right) \,. \tag{34}$$

It turns out that this function has a property which allows to minimize it very efficiently: it is a *submodular function*.

Submodular Functions

The concept of a submodular function in discrete optimization appears to be in several respects analogous to that of a convex function in continuous optimization. In many combinatorial theorems and problems, submodularity is involved, in one form or another, and submodularity often plays an essential role in a proof or an algorithm. Moreover, analogous to the fast methods for convex function minimization, it turns out that submodular functions can also be minimized fast, i. e. in polynomial time.

Submodularity is a special property of *set functions*, which are defined as follows: Let V be a finite set and $2^V = \{X \mid X \subseteq V\}$ be the set of all the subsets of V. A function $f : 2^V \to \mathbb{R}$ is called a set function.

Now a set function f is **submodular** if for all subsets $A \subseteq V$ and $B \subseteq V$:

$$f(A) + f(B) \geq f(A \cap B) + f(A \cup B) \,. \tag{35}$$

It is simple to show that a function f is submodular if and only if for any subsets $S \subseteq R \subseteq V$ and for any $x \in V$:

$$f(S \cup \{x\}) - f(S) \geq f(R \cup \{x\}) - f(R) \,. \tag{36}$$

This means intuitively that adding an element to a "small" ensemble S (since $S \subseteq R$) has more effect than adding to a "large" ensemble R.

The function (34) $f_P(A) = -(c(A) + w(A))$ is submodular, because the function $-c(A)$ is submodular (and the function $w(A)$ is modular: Take two sets of edges $A \subseteq B$ and an edge e. Inspecting the three possible cases: $e \in A$, $e \notin A$ and $e \in B$, $e \notin A$ and $e \notin B$ one sees that $c(A \cup \{e\}) - c(A) \leq c(B \cup \{e\}) - c(B)$, which is the reverse of (36), so that the function $-c$ is a submodular function. Note that $c(E')$ with $E' \subseteq E$ counts the number of connected components of the graph G' that contains *all* vertices V of the complete graph but only the edges in E'. Thus adding an edge will never increase the number of components.

On the other hand it is straightforward to see that the function $w(G) = \sum_{e \in G} w_e$ verifies $w(A \cup C) + w(A \cap C) = w(A) + w(C)$. It is a so-called *modular* function. Consequently the function (34) f_P is a submodular function. In summary we are looking for the sets of edges minimizing the submodular function f_P for which a *strongly polynomial* algorithm has been recently discovered.

In passing we note that we encountered other examples of submodular functions already in the preceding sections, namely the function that defines the costs of cuts in a graph with positive edge weights, which occurs the interface problem and the random field Ising model in the last sections: Take a graph $G = (V, E)$ and define C to be a function of the subsets of the V and $C(U \subseteq V)$ is the

number of edges having exactly one end in U. This function can be generalized to the case where the edges are directed and weighted, i. e. each edge carries an arrow and a positive number. The function $C(U \subseteq V)$ is then the sum of the weight of the edges having the beginning vertex in U and the ending vertex not in U. This kind of function is generally called a "cut" and is submodular.

Minimization of Submodular Function

The minimization of any submodular function can be done in polynomial time. This was first published in reference [54] in 1981. In this paper the authors utilize the so-called ellipsoid method. However this method is not a combinatorial one and is far from being efficient. In that respect this result was not quite satisfactory at least for the practical applications. Eighteen years later, Iwata–Fleischer–Fujishige [55], and independently Schrijver [56] discovered a combinatorial method which is fully satisfactory from the theoretical, as well as from the practical, point of view.

The general method uses a mathematical programming formulation. The problem is algebraically expressed as a linear program, i. e. a set of variables y_S associated to each subset $S \subset V$ is introduced , these variables are subjected to constraints and a linear function F of these variables is to be minimized. The constraints include a set of linear equations and the condition that each of the y_S is zero or one. This last condition is in general extremely difficult to realize. However, it turns out that a theorem due to Edmonds [57] indicates this condition can be simply dropped, and that automatically the set of values y_S which minimize F will all be zero or one! Actually only one variable $y_{S^\star} = 1$ will be non zero and it is precisely associated to the optimal set. Combined with the dual version of this linear program, it provides a characterization of the optimal set.

The general algorithm mentioned above can be applied to minimize (34), however, due to the specific form of the function to minimize, a more suitable method does exist. For this a property that is true for any submodular function is useful. To emphasize that the function f to minimize is defined on all the subsets of a set E we will label f with the index E as f_E. Let us now consider a subset $F \subseteq E$; one can define a set function on F by $f_F(A) = f_E(A)$ for any $A \subseteq F$. If the function f_E is submodular then its restriction f_F is also submodular. We have the following property:

Let $F \subseteq E$ and $e \in E$, if A_F is an optimal set of the set function f_F defined on F, then there will be an optimal set $A_{F\cup\{e\}}$ of the function $f_{F\cup\{e\}}$ defined on $F \cup \{e\}$ such that $A_F \subseteq A_{F\cup\{e\}}$.

To make the notation simpler we denote the function $f_{F\cup\{e\}}$ on $F \cup \{e\}$ by f_1. Let A be an optimal set of f_F on F and B an optimal set of f_1 on $F \cup \{e\}$. One has

$$f_1(A \cup B) \leq f_1(A) + f_1(B) - f_1(A \cap B) \tag{37}$$

since f_1 is submodular. But $f_1(A) = f_F(A)$ and $f_1(A \cap B) = f_F(A \cap B)$ since both A and $A \cap B$ are in A. Since A is an optimal set one has $f_F(A) \leq f_F(A \cap B)$ and consequently $f_1(A) - f_1(A \cap B) \leq 0$. Inserting this last inequality into (37) one finds that $f_1(A \cup B) \leq f_1(B)$ which proves that $A \cup B$ is one of the optimal sets (Q.E.D.).

This property has an important consequence. Indeed let us suppose that the optimal set has been found for a subset F of E. Then all the elements of E which have been selected as belonging to the optimal set of F will still belong to one optimal set of all the sets $G \supseteq F$. In other words, let us find the optimal set for $\{e_0, e_1\}$ where e_0 and e_1 are *arbitrary* elements of E; then if we find that any of these two elements belongs to the optimal set, it will belong to one optimal set for $F \subseteq E$! Such an algorithm which makes a definitive choice at each step is called a *greedy* algorithm.

Based on this observation an efficient algorithm for the minimization of (34) was developed in [59], see also [60].

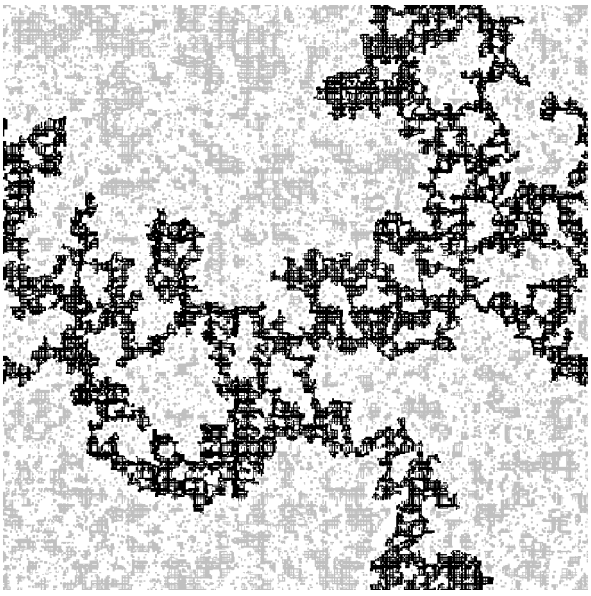
Results

The algorithm based on the ideas mentioned before and presented in detail in [59,60], was applied to various two dimensional and three dimensional lattices. A realization of the disorder is chosen accordingly to a probability distribution. In practice all the weights $w(e)$ on the edge e are rational numbers with a common integer denominator q. In other words, we choose an integer $p(e)$ for each edge and set $w(e) = p(e)/q$. To work only with integers one maximizes the product qf:

$$qf(A) = qC(A) + \sum_{e\in A} p(e)\,.$$

It is clear that if q is small compare to all the $p(e)$, then all the weights $w(e)$ will be large and the optimal set will be the set of all edges. On the contrary if q is large all the weights will be small and the optimal set will be empty. These two situations are easy to handle. Between this two limits the optimal set grows, and for a precise value q_c of q, which depends on the lattice, the optimal set percolates. This value corresponds to a phase transition. Depending on the lattice under consideration and on the distribution of the random variables $p(e)$ this transition can be first or second order.

In Fig. 8, one optimal set is shown for a lattice where each edge carries a weight 1/6 or 5/6 with probability one half (i. e. it is a critical point). The edges from the optimal



Optimization Problems and Algorithms from Computer Science, Figure 8
A 512 × 512 lattice. The edges of the optimal set belonging to the percolating cluster are shown in *black*, and the edges of the optimal set not belonging to the optimal set are in *gray* (from [60])

set belonging to the percolation cluster are shown in black, while the others are shown in gray. The percolation cluster, which is the largest connected component in the optimal subgraph $G' \subseteq G$ is fractal with a fractal dimension $d_f = 1.809$ that is related to the critical exponent $x = \beta/\nu$ for the magnetization of the random bond $q \to \infty$ Potts model (31) in two dimensions via $x = 2 - d_f = 0.191$. Surprisingly this agrees within the error bars with the magnetization exponent $x = (3 - \sqrt{5})/4$ of the random transverse Ising chain [62], which is a one-dimensional quantum spin model. A discussion of this observation and details of the computations can be found in [61].

Future Directions

We have reviewed several applications of polynomial optimization algorithms from computer science to disordered systems in statistical physics. They were used extensively in the recent years to compute numerically universal properties like critical exponents, domain wall exponents and geometrical features like roughness and stiffness with much higher precision than with Monte-Carlo methods, which suffer notoriously from equilibration problems. A number of important issues, which were controversially debated within different analytical could be clarified, numerically, in this way – as for instance the nature of the low temperature phase of the superrough phase in the two-dimensional Bragg glass [19,63], the absence of a stable glass phase in the strongly screened vortex glass model [21] and the issue of many states in various two-dimensional glassy models [64]. Other questions still remain to be answered, as for example the phenomenon of an apparent non-universality in the three-dimensional random field Ising model [65].

NP-hard problems occurring in the statistical physics of disordered systems, still remain a challenge: Examples are the computation of ground states of spin glass models on non-planar graphs, like the three-dimensional spin glass or the random field Potts model for three or more Potts states [66]. Stochastic optimization techniques like hysteretic optimization [67] or extremal optimization [68] have reached a high level of sophistication but naturally suffer from the lack of a proof of optimality of the resulting solution. Progress in the development of exact and efficient algorithm that can handle sufficiently large system sizes to perform a reliable finite size scaling analysis is being made [47] and highly rewarding.

The cross-fertilization between computer science and statistical physics is also fruitful in the other direction: Phase transitions that occur in some combinatorial optimization problems like the satisfiability problem (SAT) were studied intensively in recent years by physicists and remarkable progress has been achieved in understanding it and inventing efficient algorithms. These developments were not covered in this article, excellent introductions can be found in [69].

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