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LETTER TO THE EDITOR

Using network-flow techniques to solve an optimization problem from surface-physics

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Abstract. The solid-on-solid model provides a commonly used framework for the description of surfaces. In recent it has been extended in order to investigate the effect of defects in the bulk on the roughness of the surface. The determination of the ground state of this model leads to a combinatorial problem, which is reduced to an uncapacitated, convex minimum-circulation problem. We will show that the successive shortest path algorithm solves the problem in polynomial time.

1. Introduction

In the past twenty years there has been a fruitful collaboration between theoretical physicists and researchers from the field of combinatorial optimization on the determination of the global energy-minimum (ground state) in various spin-glass models. The observation that the ground state of the Ising model can be found by solving an certain max-cut problem, has drawn the attention of physicists to the methods developed in graph theory [1]. Conversely this application has stimulated research into the max-cut problem itself [2, 3]. It the same spirit it has been shown that the max-flow problem arises in the context of the random-field Ising model [4].

The *solid-on-solid (SOS) model*, on which we will comment here, is a microscopic approach to the description of the aggregation of atoms on a crystalline substrate. In contrast to the above mentioned Ising models, where the dynamic variables can take on only two values, in the SOS model these variables are integer valued. At first sight this fact seems to complicate the optimization problem. However, as with the Ising model, the underlying structure can be represented by a graph. We will show in this letter that in the planar case the problem of minimizing the surface energy can be reduced to the problem of finding a network circulation that minimizes a convex objective function.

The growth of surfaces is a subject of intense research in chemistry and solid state physics. A deeper understanding of the relevant processes has applications in the fabrication of semiconductors and various other fields where the precise shape of the surface is crucial [5]. In the simple approach taken by the SOS model the lattice structure of real crystals is taken into account by subdividing the surface into discrete sites (e.g., unit squares) on which particles, modelled by unit cubes, can aggregate [6, 7]. There are several possible parametrizations of the model. The one which is commonly used for theoretical investigations yields the surface energy

$$H(h) = \sum_{\langle ij \rangle} (h_i - h_j)^2. \tag{1}$$

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Here $h_i \in \mathbb{Z}$ is the height of the surface at site i and $\langle ij \rangle$ indicates all pairs of nearest neighbour sites on e.g. a square lattice, mimicking the crystalline structure. Obviously the ground state of this model is flat, i.e. $h_i =$ constant for all i. Thermal fluctuations lead to a roughening transition at some temperature above which the height–height correlation function increases logarithmically with the distance.

One assumption of this model is the flatness of the underlying substrate, i.e. a bulk-ordered crystal. Due to the presence of quenched defects one should consider the intriguing question of what the effect of a disordered substrate on the thermodynamic (and non-equilibrium growth) properties of the surface might be [8]. It has been suggested [9] that a disordered substrate be introduced into the model (1) by providing each of the height variables with a real-valued offset $d_i \in \mathbb{R}$, which is generally chosen to be from $[-0.5, 0.5]$:

$$h_i := n_i + d_i \qquad \text{with} \quad n_i \in \mathbb{Z}. \tag{2}$$

This model has some new features not contained in the original one. The influence of the disorder tends to roughen the surface *also at low temperatures*. In particular a new phase has been predicted [9, 10], where height–height correlations diverge more strongly with the distance than logarithmically. Since this is a low-temperature phase the properties of the ground state of (1) with (2), which is no longer trivial due to the competition between the elastic term $(h_i - h_j)^2$ and the random offsets d_i, are of crucial interest.

The letter is organized as follows. Section 2 introduces the reduction to a convex network-flow problem and in section 3 we will then show that (1) can be minimized in strictly polynomial time using the techniques introduced in [11]. We use standard notation from graph theory, and refer the reader to [12] for the definitions.

2. Reduction to a network-flow problem

Let $D = (V, E)$ be a directed graph. The optimization problem we consider is

$$\min H(n) = \sum_{(ij)\in E} ((d_i + n_i) - (d_j + n_j))^2 \qquad \text{s.t.} \quad n_i \in \mathbb{Z} \quad \text{for all} \quad i \in V. \tag{3}$$

Using the definitions $d_{ij} := d_i - d_j$ and $x_{ij} := n_i - n_j$ the objective function can be written as

$$H(X) = \sum_{(ij)\in E} (d_{ij} + x_{ij})^2. \tag{4}$$

We intend to reformulate the original optimization problem in terms of the variables x_{ij}. Obviously we must demand $x_{ij} \in \mathbb{Z}$ for all edges $(ij) \in E$. Furthermore, since the x_{ij} describe potential differences in the scalar field given by a set of height variables n_i, it is clear that the sum of the x_{ij} along any oriented cycle on the surface has to be zero. The following theorem establishes this constraint formally in the special case, where D is a planar graph.

Theorem 1. Let $D = (V, E)$ be a planar, directed graph and $D^* = (V^*, E)$ be the associated dual graph. There exists a set of node-variables $n_1, \ldots n_{|V|}$ such that $X = (x_{ij})^E = (n_i - n_j)^E$ if and only if X satisfies

$$\sum_{(ij)\in E} x_{ij} - \sum_{(ji)\in E} x_{ji} = 0 \qquad \text{for all dual nodes} \quad i \in V^*. \tag{5}$$

A proof of this theorem can be found in [12, chapter 5].

Given a vector X and a node i we call the number

$$g_i(X) := \sum_{(ij)\in E} x_{ij} - \sum_{(ji)\in E} x_{ji}$$

the excess of a node i. A complete formulation, which, for planar graphs, is equivalent to (3) is thus given by

$$\min H(X) = \sum_{(ij)\in E} (d_{ij} + x_{ij})^2 \tag{6}$$

s.t.

$$x_{ij} \in \mathbb{Z} \qquad \text{for all edges } (ij) \in E \tag{7}$$

$$g_i(X) = 0 \qquad \text{for all dual nodes } i \in V^*. \tag{8}$$

A vector X satisfying these equations is called a circulation [13]. The problem is a convex network-flow problem in the dual graph without any capacity constraints (the flow-variables x_{ij} on each edge can take on arbitrary positive or negative values). We note that this reduction, as well as the results in the following section, more generally hold for any objective function, which can be written as

$$H(X) = \sum_{(ij)\in E} \theta_{ij}(x_{ij})$$

where the θ_{ij} are convex functions with a minimum.

3. Algorithm and complexity

The algorithms which solve the convex flow problem [11] are not strictly polynomial if there are no capacity constraints. We will show in this section that in the special case of problem (6) the time complexity of the successive shortest path algorithm for convex flow can be bounded by a strict polynomial. For this purpose we start with a brief review of the algorithm, a more detailed description can be found in [13].

The underlying philosophy is to search for the solution in a subset of $\mathbb{Z}^E$, in which each vector X yields a lower bound for the optimum of (6) but does not necessarily satisfy the flow-constraints (8). The flow balance at all nodes has to be approached iteratively by the algorithm. To characterize this subset, one introduces the notion of dual feasibility:

Definition 1. Let $H(X) = \sum_{(ij)\in E} \theta_{ij}(x_{ij})$ be a sum of functions $\theta_{ij}(x)$ of the components x_{ij} of X. A vector X is called dual feasible, if there is a number π_i for every node (potential function), such that for all edges $(ij) \in E$ the reduced-cost inequalities

$$\begin{aligned} c^{\pi}_{ij}(x_{ij}) &:= \theta_{ij}(x_{ij}+1) - \theta_{ij}(x_{ij}) - \pi_j + \pi_i \geqslant 0 \\ c^{\pi}_{ji}(x_{ij}) &:= \theta_{ij}(x_{ij}-1) - \theta_{ij}(x_{ij}) + \pi_j - \pi_i \geqslant 0 \end{aligned} \tag{9}$$

are satisfied.

Theorem 2. Let X be a dual feasible vector and let X_{opt} be an optimal solution of problem (6), then $H(X) \leqslant H(X_{\text{opt}})$.

The proof is given in [13, chapters 9 and 14.3]. An immediate consequence of this theorem is:

Corollary 1. A dual feasible vector X satisfying (7), (8) is an optimal solution of problem (6).

In order to apply the successive shortest path algorithm we determine a dual feasible initial solution. Here we can choose the vector $X_s \in \mathbb{Z}^E$, whose components minimize the functions $\theta_{ij}(x)$ and the potential function $\pi := (\pi_i)^{|V|} = 0$. Note that, when $\pi = 0$, the reduced costs (9) simply measure the change of the objective function triggered by a change of the (ij) component by plus (minus) one. These are clearly all positive if X minimizes every summand of (6).

The initial solution does in general not satisfy the flow-equations (8). The excess $g_i(X)$ of all nodes is then balanced by iteratively augmenting X along paths between supply nodes ($g_i(X) > 0$) and demand nodes ($g_i(X) < 0$), which are shortest paths with respect to the reduced costs. The variables x_{ij} associated with the edges along such a path are changed by exactly one unit (the sign depends on the orientation of the edge in the path).

Due to the non-linearity of the objective every update of X leads to a new set of arc weights. However, the convexity of the individual functions θ_{ij} ensures that the inequalities (9) still hold after every augmentation, when $c^{\pi}_{ij}(x_{ij})$ is replaced by $c^{\pi}_{ij}(x_{ij} + a)$ with $a \in \{-1, 0, 1\}$. Therefore the algorithm works correctly because it always maintains dual feasibility of X with respect to the current set of arc weights.

procedure successive shortest path
  begin
    $X = \min\{H(X) | X \in \mathbb{Z}^E\}$
    $\pi = 0$
    while there is a node s with $g_s(X) > 0$
      compute the reduced costs $c^{\pi}(X)$
      determine the shortest path distances $d(i)$ from s to all other nodes
        with respect to the reduced costs
      choose a node t with $g_t(X) < 0$
      let $w(s, t)$ denote the shortest path vector from s to t in D
      $X = X + w(s, t)$
      $\pi = \pi - d$
    end
  end

The complexity of the algorithm is $O(G(X_s))S(n, m)$. Here $S(n, m)$ is the time needed for a shortest path search in a network with positive arc weights and

$$G(X_s) := \frac{1}{2} \sum_i |g_i(X_s)|$$

counts the number of paths needed to balance the excess of all nodes. The following lemma then yields an upper bound for the value of $G(X_s)$.

Lemma 1. The vector $X_s \in \mathbb{Z}^E$ that minimizes $H(X)$ (equation(6)) satisfies $G(X_s) \leqslant |E|$.

Proof . If the integrality and flow constraints are neglected the global minimum of $H(X) = \sum_{(ij)\in E}(d_{ij} + x_{ij})^2$ is attained at $-d := (-d_{ij})^E$ with $H(-d) = 0$. If we now take into account the integrality–constraints it follows from the convexity of the $(d_{ij} + x_{ij})^2$ that the minimum $x^s_{ij} \in \mathbb{Z}$ is attained in either $\lceil -d_{ij} \rceil$ or $\lfloor -d_{ij} \rfloor$. We thus find that

$$|x^s_{ij} - (-d_{ij})| \leqslant 1.$$

From theorem 1 we obtain $G(-d) = 0$ and thus

$$G(X_s) = G(X_s) - G(-d) \leqslant \sum_{(ij)\in E} |x^s_{ij} - (-d_{ij})| \leqslant |E|. \qquad \square$$

4. Computer experiments

We implemented the successive shortest path algorithm for the convex-flow problem. The program needs less than 80 s on a Sparc Workstation to solve instances of grid graphs with 128×128 nodes and randomly chosen offsets to optimality. Grid graphs of size 200×200 nodes take about 10–15 min. We used C++ for our implementation and made use of the LEDA class library [14]. The physical results, which have been obtained with this program, together with their theoretical interpretation will be reported elsewhere.

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