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NP-hardness of the cluster minimization problem revisited

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Abstract

The computational complexity of the ‘cluster minimization problem’ is revisited (Wille and Vennik 1985 *J. Phys. A: Math. Gen.* **18** L419). It is argued that the original NP-hardness proof does not apply to pairwise potentials of physical interest, such as those that depend on the geometric distance between the particles. A geometric analogue of the original problem is formulated, and a new proof for such potentials is provided by polynomial time transformation from the independent set problem for unit disk graphs. Limitations of this formulation are pointed out, and new subproblems that bear more direct consequences to the numerical study of clusters are suggested.

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The present contribution addresses the inherent computational difficulty of finding the ground-state configuration $\mathbf{R} = (\mathbf{r}_1, \dots, \mathbf{r}_N)$ of a classical N -particle system with the total potential energy

$$U(\mathbf{R}) = \sum_{i=1}^N \sum_{j>i}^N u(|\mathbf{r}_j - \mathbf{r}_i|), \quad (1)$$

where each $\mathbf{r}_i \in \mathbb{R}^3$. Though fairly general in scope, this problem is of particular interest in the characterization of the energy landscapes of atomic clusters (see, e.g., [1, 2]), and bears important consequences to the efficiency of Monte Carlo sampling methods for clusters at low temperatures.

When addressing such fundamental aspects of optimization problems, a primary goal is to establish whether the given problem is ‘NP-hard’, a complexity class also known as *intractable* since their solution in the worst-case scenario requires a number of computational steps that increases exponentially with the ‘size’ of the problem (intractability hinges upon the validity of the $P \neq NP$ conjecture, which is nevertheless widely accepted; see [3, 4] for details, or [5] for a gentle introduction aimed at the physics audience). Establishing the membership of a problem in the NP-hard class is, on the one hand, of fundamental importance to the field of

computational complexity, for a given polynomial time solution to the problem would collapse the entire NP class into P, and on the other hand of practical interest to the problem itself, for it indicates that the chances of finding a general-purpose algorithm with polynomial efficiency across all instances of the problem are very small, thereby encouraging the development of specialized algorithms that can benefit from whatever physical insight one has into the specific instance of the problem at hand. Proofs of NP-hardness are especially welcome in light of recent efforts to characterize the boundaries between exponential and polynomial behaviour in ‘typical’ instances of NP-complete problems (see, e.g., [6–8]), an endeavour that has the potential of providing valuable guidance for dealing with NP-hard optimization problems.

A study on the computational complexity of classical systems interacting via pairwise potentials has been reported in [9], a celebrated work that is frequently cited in the literature as providing a proof that the ‘cluster minimization problem’ is NP-hard (see, e.g., [10–15]). It is part of the goal of the present work to argue that this proof is too general, and that a different proof is necessary for physically relevant potentials such as those described by equation (1) (i.e. those that depend on the geometric distance between the particles), and hence that the NP-hardness of the ‘physical’ cluster minimization problem is still an open issue. The remainder of this paper is thus divided into three parts: a critical analysis of [9], a proof of NP-hardness valid for potentials of the form of equation (1), and a discussion on the limitations of this proof.

One of the simplest ways of proving that a given problem π is NP-hard is by ‘restriction’, i.e. by showing that a specific instance of the problem π coincides with a problem π' already known to be NP-hard (much of the present discussion on computational complexity was adapted from [3]). Often times, however, the connection between the problem of interest and a known intractable problem is not immediate; in this case, one can still establish the NP-hardness of π by ‘polynomial transformation’ from π' , i.e. by showing that every instance I' of π' can be transformed to an instance $I = f(I')$ of π in polynomial time, and that a solution of I also solves I' . The NP-hardness proof of Wille and Vennik was based on such a transformation [9]: Formulating the cluster minimization problem in terms of ‘graphs’ (see, e.g., [4]), these authors considered what will be henceforth referred to as the WEIGHTED EDGE problem, showing that the TRAVELING SALESPERSON (TSP) problem can be transformed to WEIGHTED EDGE; since TSP is known to be NP-hard, so must be WEIGHTED EDGE. In the following, I will analyse the proof offered by these authors, arguing that it requires pair ‘potentials’ that are far more general than those of physical interest, which leaves the possibility that the case of more restrictive and physically relevant potentials may be treated by a polynomial-time algorithm.

First, let us state Wille and Vennik’s problem following the standard format of Garey and Johnson [3].

[WEIGHTED EDGE] *Instance:* a complete graph $G = (V, E)$, a weight function $w(e)$ for each $e \in E$, and a number $N < |V|$. *Problem:* find a subgraph $G' = (V', E')$ of size $|V'| = N$ such that

$$\sum_{e \in E'} w(e) \text{ is minimal.}$$

Here a complete graph $G = (V, E)$, where V are the vertices and E are the edges connecting the vertices, is one in which every pair of vertices is connected by an edge (i.e. a ‘clique’), and the notation $|V|$ indicates the number of vertices. An illustration of this problem is provided in figure 1.

When formulating the cluster minimization problem as WEIGHTED EDGE, the authors of [9] had in mind the following analogy: V is the set of ‘sites’ that the N particles are allowed

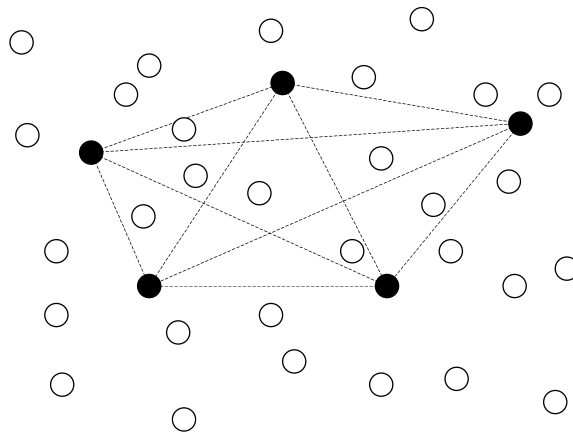


Figure 1. An illustration of the WEIGHTED EDGE problem, with vertices represented by circles and edges by dotted lines. The problem is to choose N out of all the vertices such that the sum of the corresponding edge weights $w(e)$ is minimal. Although the entire graph is complete, for clarity of illustration only edges connecting the vertices of a hypothetical solution with $N = 5$ are shown.

to occupy, and for every pair of sites with edge $e = (v_i, v_j)$, the function $w(e) = w(v_i, v_j)$ measures the strength of the interaction between two hypothetical particles placed in these sites. The set V is of course discrete, reflecting the discretization of the problem that accompanies any computational method, but note that no specific structure is given to either V or $w(e)$ (this arbitrariness will be discussed later in the text).

As already mentioned, the proof that WEIGHTED EDGE is NP-hard was provided in [9] by showing that it ‘contains’ TSP, more precisely by showing that there exists a weight function $w(e)$, a choice of $|V|$ as a function of N , and a labelling of the vertices in terms of pairs of ‘cities’, such that a solution of WEIGHTED EDGE would yield a minimum TSP tour¹. Though not stated in [9], it is easy to check that this labelling and choice of $w(e)$ can be done in polynomial time given any instance of TSP. One additional observation not explicitly mentioned by Wille and Vennik is that, since the NP-hardness of TSP means that worst-case solutions to the problem are found in time exponential in the number of *cities*, their result implies only that worst-case solutions to WEIGHTED EDGE are found in time exponential in the number of *sites*, not in the number of particles N as one would like to show (recall that the general instance of WEIGHTED EDGE does not tie $|V|$ to N). Nonetheless, it stands to reason that any algorithm relevant to the cluster minimization problem will adjust the size of V so as to ensure comparable spatial resolutions for clusters of different sizes, and a reasonable choice would be a polynomial in N , i.e. $|V| \propto N^p$ for some integer $p > 0$. Thus, the NP-hardness of WEIGHTED EDGE with this additional property says that the completion time of any algorithm that solves the problem will indeed scale exponentially with the number of particles N .

Finally, observe that the choice of $w(e)$ that allows the connection with TSP (equation (4) in [9]) is too general to reflect physical problems of interest; in particular, it requires the possibility that the ‘potential’ between two sites depends on *each individual site* in question,

¹ A more direct proof that WEIGHTED EDGE is NP-hard can be given. Indeed, given any graph $G^* = (V^*, E^*)$, construct a complete graph $G = (V^*, E)$, setting $w(v_i^*, v_j^*) = 1$ if there is a corresponding $(v_i^*, v_j^*) \in E^*$, and $w(v_i^*, v_j^*) = 2$ otherwise. The solution of WEIGHTED EDGE for the graph thus constructed has a total weight equal to $N(N-1)/2$ if and only if G^* contains a clique of size N , and the foregoing transformation can be done in polynomial time. But determining if a graph contains a clique of a given size is known to be an NP-complete problem (CLIQUE, see [3]), and thus WEIGHTED EDGE must be NP-hard. QED

and not just on their relative geometric distance. Although the authors state that their proof remains true for spherically symmetric potentials ‘by comparing it to the general and the Euclidean travelling salesperson problem’ [9], this is far from clear: it is difficult to imagine a polynomial time transformation from a generic instance of the (Euclidean or not) TSP problem to an instance of the *geometric* WEIGHTED EDGE problem, where the vertices are points in the Euclidean space and the weights $w(e)$ are geometric distances (see CLUSTER MINIMIZATION below). The proof of the Euclidean TSP that the authors refer to is quite elaborate, and requires methods other than simple restriction [16], and it is also not clear how this proof generalizes to their problem. In the following, an explicit proof for potentials that depend on the geometric distance between the particles will be provided.

The problem of minimizing the energy of N particles with spherically symmetric pairwise interaction can be stated as

[CLUSTER MINIMIZATION] *Instance:* a set of sites S in \mathbb{R}^3 , a number of particles $N < |S|$, and a potential function $u(r)$. *Problem:* find a subset $S' = \{\mathbf{r}_1, \dots, \mathbf{r}_N\}$ of S with size $|S'| = N$, such that

$$\sum_{i=1}^N \sum_{j>i}^N u(|\mathbf{r}_j - \mathbf{r}_i|) \text{ is minimal.}$$

Before we proceed, note the crucial difference with respect to WEIGHTED EDGE: in CLUSTER MINIMIZATION, it is the *relative geometric position* of the sites that determines the strength of the interaction potential. The proof of [9] for the WEIGHTED EDGE problem does not apply here, and likewise there are several subproblems of WEIGHTED EDGE not amenable to that proof which are nevertheless NP-hard by restriction to CLUSTER MINIMIZATION (e.g. the case where the interaction depends on the vectorial distance, $u = u(\mathbf{r}_j - \mathbf{r}_i)$, can clearly be restricted to spherically symmetric potentials).

It will now be shown that the unit disk graph (UDG) problem UDG INDEPENDENT SET, a decision problem known to be NP-complete [17], can be transformed to CLUSTER MINIMIZATION in polynomial time. The problem can be stated as

[UDG INDEPENDENT SET] *Instance:* a set D of disks of unit radius in \mathbb{R}^2 , and an integer $K < |D|$. *Problem:* does D contain an independent set of size K , i.e. a subset D' of D with K disks such that the disks never overlap with each other?

The problem UDG INDEPENDENT SET is one among various graph-theoretic problems that remain intractable when the graphs are restricted to be of the unit disk type, i.e. when vertices can be represented by disk centres, and edges by causing the corresponding disks to overlap in space [17] (see the illustration in figure 2). The problem of determining whether an arbitrary graph can be represented by a unit disk graph is also NP-complete [18], and so far the only interesting problem in this context that allows a polynomial time solution seems to be UDG CLIQUE [17].

The proof proceeds by choosing the sites S of CLUSTER MINIMIZATION to coincide with the centre of the disks D of a given instance of UDG INDEPENDENT SET (this can clearly be done in polynomial time, and effectively places the sites in a plane), and setting

$$u(r) = \begin{cases} 2, & \text{for } (r \leq 1) \\ 1, & \text{for } (r > 1). \end{cases}$$

Therefore, this instance of CLUSTER MINIMIZATION has a solution with total energy equal to $N(N - 1)/2$ if and only if D has an independent set with N disks. In other words, an answer to UDG INDEPENDENT SET is immediately available from a solution of the corresponding

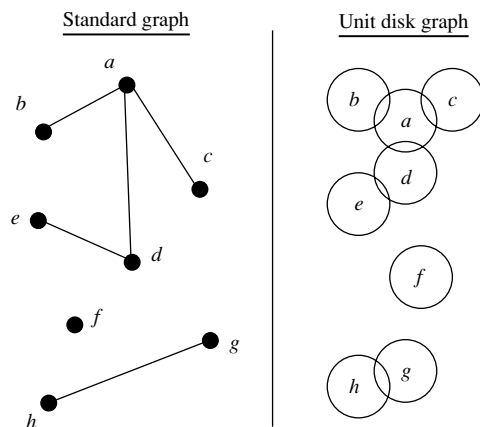


Figure 2. An illustration of a unit disk graph. Left: a graph drawn in the ‘standard’ format; Right: the corresponding UDG. Note that the problem of determining whether an arbitrary graph can be represented as a UDG is itself NP-hard [18].

CLUSTER MINIMIZATION problem (recall that the evaluation of the energy of an N -particle system interacting with pairwise potentials can be done in polynomial time, more explicitly in $\mathcal{O}(N^2)$ steps). Thus, since UDG INDEPENDENT SET is NP-complete, it must be that CLUSTER MINIMIZATION is an NP-hard problem. (Note the similarity of this argument to that used to show that HAMILTONIAN CIRCUIT can be transformed to TSP in [3, pp 35–6].)

The above formulation of the cluster minimization problem is subject to some caveats. As already discussed in the case of WEIGHTED EDGE, the assumption that the total number of sites $|S|$ grows with the number of particles N is required in order to have an intractability result in terms of N . A more subtle limitation of the present formulation can be appreciated by stating the foregoing proof in words: *given an arbitrary set of sites in \mathbb{R}^3 and a spherically symmetric but otherwise arbitrary pair-potential energy function $u(r)$, no algorithm can find the minimum energy configuration of the system in time bounded by a polynomial in the number of particles N .* (As usual, this result hinges upon the $P \neq NP$ conjecture, see the introductory paragraphs above.) This is perhaps not the most relevant result for the cluster minimization problem, since in practice one seldom uses a discretization different from the simple cubic lattice (this happens, e.g., when the components of \mathbf{r} are represented by finite-precision, binary numbers). Ideally, one would like to show that for any ‘reasonable’ discrete representation of the continuum (see, e.g., [19] for a formalization and examples of this concept), the arbitrariness in the choice of $u(r)$ by itself is sufficient to make the problem NP-hard, i.e. that for any such lattice, there are choices of $u(r)$ leading to intractable solutions. The foregoing proof of course fails when the sites are arranged in a simple cubic structure, for the existence of an independent set of a given size in this case is straightforwardly determined by the radius of the disks and the lattice spacing. In fact, it is known that a polynomial time algorithm exists for finding independent sets in unit disk graphs restricted to ‘grid’ structures [17]. The NP-hardness of this subproblem seems considerably more difficult to prove than the more general CLUSTER MINIMIZATION problem introduced in this study, and would certainly be a welcome result in the literature.

In summary, a critique of the celebrated NP-hardness proof of the cluster minimization problem [9] was offered, showing that a separate proof is necessary when the pairwise potential is a function of the geometric distance between the particles only. Using a geometric

generalization of the formulation adopted in [9], an independent proof for such cases was presented by transformation from the independent set problem for unit disk graphs [17]. Limitations of this new proof were discussed in the last paragraph, and a subproblem that fixes the lattice structure was suggested as being more relevant to traditional numerical implementations of the cluster minimization problem. To this author's knowledge, however, the intractability of this subproblem remains unknown.

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