Auxetic deformations and elliptic curves

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Abstract

In materials science and engineering, auxetic behavior refers to deformations of flexible structures where stretching in some direction involves lateral widening, rather than lateral shrinking. We address the problem of detecting auxetic behavior for flexible periodic bar-and-joint frameworks. Currently, the only known algorithmic solution is based on the rather heavy machinery of fixed-dimension semi-definite programming. In this paper we present a new, simpler algorithmic approach which is applicable to a natural family of three-dimensional periodic bar-and-joint frameworks with three degrees of freedom. This class includes most zeolite structures, which are important for applications in computational materials science. We show that the existence of auxetic deformations is related to properties of an associated elliptic curve. A fast algorithm for recognizing auxetic capabilities is obtained via the classical Aronhold invariants of the cubic form defining the curve. A related alternative is also considered.

Keywords: periodic framework; auxetic deformation; elliptic curve; Aronhold invariants; zeolites.

1. Introduction

In this paper we study a geometric problem originating in materials science. The main result is an efficient algorithm for detecting *auxetic behavior* in generic three-dimensional periodic bar-and-joint frameworks with independent edge constraints and three degrees of freedom. The method has

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immediate applications to frameworks of vertex-sharing tetrahedra, which include the important family of crystalline materials known as zeolites.

Motivation: auxetic behavior in materials science. When a physical material is stretched along an axis, its "typical" response is a lateral shrinking. Yet this behavior is not universal: certain natural or man-made materials have the rather counter-intuitive property of widening rather than shrinking. This type of "growth" has been called *auxetic behavior* [17]. In elasticity theory, Poisson's ratio for two orthogonal directions **a** and **b** is defined as the signed ratio of the lateral effect along **b** to the extension along **a** due to uniaxial tension applied in that direction. For "typical" materials the Poisson's ratio is taken with a positive sign, while materials with auxetic behavior are said to have negative Poisson's ratios [18, 19, 22, 23, 24]. The difference is often illustrated in the literature with the two-dimensional periodic bar-and-joint *honeycomb* examples shown in Fig. 1.

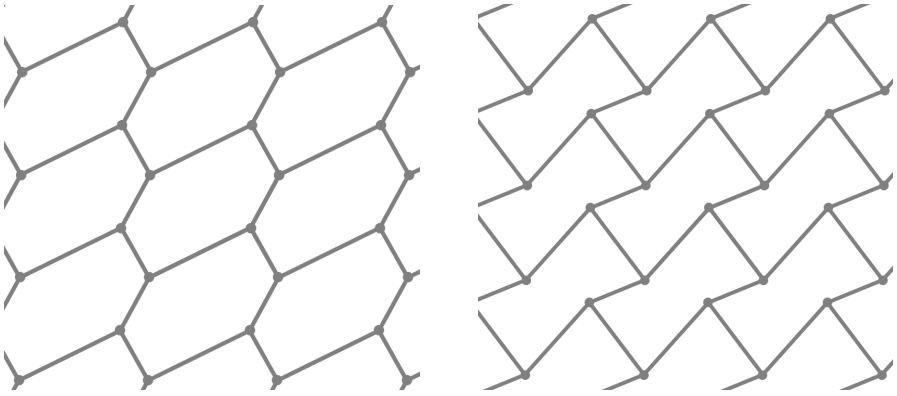

Figure 1: (Left) The *regular honeycomb* has positive Poisson's ratios, while the *re-entrant honeycomb* (right) exhibits auxetic behavior.

In mineralogy, the "rigid unit mode" approach to displacive phase transitions in crystalline materials relies on the periodic framework structure at the atomic level [15]. In this context, auxetic behavior was observed for cristobalite [37] and conjectured among zeolites [20, 34]. For cellular and periodic materials, the importance of the underlying geometry has been frequently emphasized [25, 28, 29]. However, the approach via determinations of Poisson's ratios has produced only a limited catalog of structures capable of auxetic behavior [16, 24]. Currently, with new and augmented possibilities for digital fabrication (3D printing) and an increased interest in mechanical

metamaterials, geometric structural design has reached a pivotal role and position [2, 33].

In our recent work [9], we laid the foundations of a strictly geometric theory of auxetic deformations for periodic bar-and-joint frameworks. Auxetic behavior is recognized based on the evolution of the periodicity lattice along one-parameter trajectories. As reviewed after this introduction, the hallmark of an auxetic trajectory is that the Gram matrix of a basis of periods traces a curve of symmetric matrices with all tangent directions contained in the positive semidefinite cone. This purely geometric approach has uncovered new principles for auxetic design [11, 12] and has opened the door to rigorous mathematical techniques. Design and recognition of auxetic features may be considered the obverse and reverse of the auxetic coinage.

Main theoretical result: overview. In this paper, we investigate the auxetic capabilities of a natural class of three-dimensional periodic frameworks, which includes many structures of interest in mineralogy and materials science, such as silica and zeolites [27]. Specifically, we address the following problem.

Problem 1 (**Identify auxetic capability).** *Let $\mathcal{F}$ be a 3D periodic bar-and-joint frameworks with independent edge constraints, n vertex orbits, $m = 3n$ edge orbits and hence three degrees of freedom. Decide if $\mathcal{F}$ allows strictly auxetic local trajectories.*

As it is often the case with similar questions in rigidity theory and kinematics, we assume certain genericity conditions on the framework (they will be stated explicitly in Section 4). In practice, most tetrahedral crystal frameworks would satisfy our conditions, which guarantee that local deformations are represented by variations of the periodicity lattice and the three dimensional tangent space at the initial configuration is in general position.

The connection with elliptic curves indicated in the title comes from restricting the determinant function on symmetric 3×3 matrices to such a three-dimensional vector subspace. The genericity condition will imply that the resulting ternary cubic form defines a non-singular projective curve. The most remarkable theoretical fact is that our question about auxetic capabilities of the periodic framework turns into a question about the real points of an elliptic curve.

Main algorithmic result: overview. Our formulation of auxetic behavior leads to significant connections with convex algebraic geometry, spectrahedra and semidefinite programming, as already noted in [9], Corollary 7.1. In particular, deciding infinitesimal auxeticity for a d-periodic bar-and-joint framework can be formulated as a semi-definite program (SDP) in fixed-dimension d, for which polynomial time solutions exist [31][1]; see also [26] for a recent survey on the related topic of low-rank SDP. Using the new connections with elliptic curves presented in this paper, we can avoid the SDP machinery for the family of n-vertex, $3n$-edge orbit periodic frameworks. Specifically, classical results on the Hesse form of a cubic, Aronhold invariants and the modular J-invariant [3, 14, 35] lead to a simpler and cleaner decision algorithm. The main steps of the algorithm involve solving an under-constrained linear system with $3n$ linear equations in $3n+3$ unknowns, along with several algebraic calculations on cubic polynomials.

In the last section we discuss two algorithmic alternatives: one based on cylindrical decomposition and sample points on all connected components of an affine semi-algebraic set [1], the other based on smallest rank points on spectrahedra [21]. Nevertheless, our emphasis remains attached to the fuller geometrical understanding which can be obtained in the regular case via the Hesse form of the cubic. This may serve wider inquiries on variations of auxetic cones in large deformations.

Related Work. In [10], we defined and studied the stronger concept of *expansive deformation path* for a periodic framework, and proved that it is necessarily an auxetic path. For two-dimensional frameworks, we gave a complete combinatorial characterization (based on periodic pseudo-triangulations) of those frameworks that admit expansive deformations [10, 8]. This leads, in particular, to an infinite family of planar periodic auxetic mechanisms. For arbitrary dimensions, our design principles [11, 12] and connections with convex algebraic geometry bring new significance to classification problems for spectrahedra, as pursued in [30]. Also related are classical results on ternary quartic forms [32].

Frameworks with $m = 3n$ and the vertex-sharing tetrahedral structures. The three-dimensional frameworks studied in this paper have n vertex

[1]However, as pointed out to us by Anthony Man-Cho So, this remains a purely theoretical result: no implementation of the algorithm [31] is available and in practice one would have to rely on some general SDP code, such as the CVX package in MATLAB.

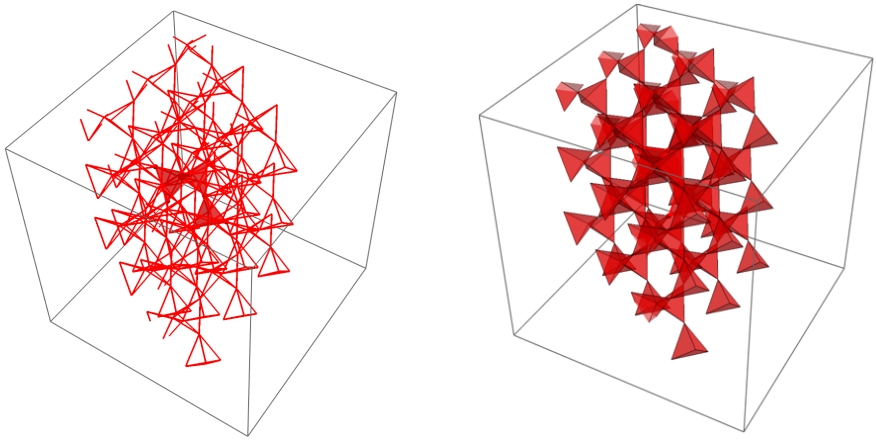

Figure 2: The quartz framework is an example of a tetrahedral 3D periodic structure. It has $n = 6$ vertex orbits and $m = 3n = 18$ edge orbits. The bar-and-joint framework is shown on the left. The edges of the three highlighted tetrahedra provide the 18 representatives for the edge orbits. In [9], we show that the path of the phase transition from low to high quartz is auxetic.

orbits and $m = 3n$ edge orbits. We assume independent edge constraints and this implies a smooth three-dimensional local deformation space, i.e. three degrees of freedom. This choice is not accidental. In general, for arbitrary dimension d, the class of periodic frameworks with n vertex orbits and $m = dn$ edge orbits has distinctive mathematical properties; for instance, the invariance of the ratio $m/n = d$ under relaxations of periodicity. A special family in dimension two is the family of pointed pseudo-triangulations. Another important family, in arbitrary dimension d, consists of periodic frameworks made of (1-skeleta of) "vertex-sharing simplices"; every vertex is common to exactly two simplices. The 3D case of vertex-sharing tetrahedral structures includes a wealth of crystal structures studied in mineralogy, such as silicates and zeolites. Quartz, for instance, is a silicon dioxide with oxygen atoms forming a tetrahedral framework as illustrated in Fig. 2. Its auxetic properties, established in [9], motivated us to seek the general decision procedure presented in this paper.

2. Periodic frameworks and deformations

In this section we review the necessary concepts related to periodic frameworks and deformation spaces. The main references are [4, 5, 7].

Periodic graphs, vertex and edge orbits. A d-periodic graph is a pair (G, Γ), where $G = (V, E)$ is a simple infinite graph with vertices V, edges E and finite degree at every vertex, and $\Gamma \subset Aut(G)$ is a free Abelian group of automorphisms which has rank d, acts without fixed points and has a finite number of vertex (and hence, also edge) orbits. The group Γ is thus isomorphic to $\mathbb{Z}^d$ and is called the *periodicity group* of the periodic graph G. Its elements $\gamma \in \Gamma \simeq \mathbb{Z}^d$ are referred to as *periods* of G. We assume V to be connected and denote by $n = |V/\Gamma|$ the number of vertex orbits and by $m = |E/\Gamma|$ the number of edge orbits.

Placements and frameworks. A periodic placement (or simply placement) of a d-periodic graph (G, Γ) in $\mathbb{R}^d$ is defined by two functions: $p : V \to \mathbb{R}^d$ and $\pi : \Gamma \hookrightarrow \mathcal{T}(\mathbb{R}^d)$, where p assigns points in $\mathbb{R}^d$ to the vertices V of G and π is a faithful representation of the periodicity group Γ, that is, an injective homomorphism of Γ into the group $\mathcal{T}(\mathbb{R}^d)$ of translations in the Euclidean space $\mathbb{R}^d$, with $\pi(\Gamma)$ being a lattice of rank d. These two functions must satisfy the natural compatibility condition $p(\gamma v) = \pi(\gamma)(p(v))$.

A placement (p, π) which does not allow the end-points of any edge to have the same image defines a *d-periodic bar-and-joint framework* $\mathcal{F} = (G, \Gamma, p, \pi)$ in $\mathbb{R}^d$, with edges $(u, v) \in E$ corresponding to bars (segments of fixed length) $[p(u), p(v)]$ and vertices corresponding to (spherical) joints. An example in dimension $d = 3$ is given in Fig. 3. Two frameworks are considered equivalent when one is obtained from the other by a Euclidean isometry.

Deformation space. Given a d-periodic framework $\mathcal{F} = (G, \Gamma, p, \pi)$, the collection of all periodic placements of (G, Γ) in $\mathbb{R}^d$ which maintain the lengths of all edges is called the *realization space* of the framework. After factoring out equivalence under Euclidean isometries, we obtain the *configuration space* of the framework (with the quotient topology). The *deformation space* is the connected component of the configuration space which contains the initial framework. Examples can be found in [4, 6].

Factoring out the Euclidean isometries. A convenient way to factor out equivalence under Euclidean isometries is to use coordinates relative to a basis given by generators of the periodicity lattice and to retain the metric information via the Gram matrix of the chosen basis. The procedure is described in [7], Section 4, and will be recalled here concisely.

After choosing an independent set of d generators for the periodicity group Γ, the image $\pi(\Gamma)$ is completely described via the $d \times d$ matrix Λ with column vectors $(\lambda_i)_{i=1,\cdots,d}$ given by the images of the generators under π. The Gram matrix for this basis will be $\omega = \Lambda^t \cdot \Lambda$.

Let us fix now a complete set of vertex representatives $v_0, v_1, ..., v_{n-1}$ for the n vertex orbits of (G, Γ). The framework $\mathcal{F}$ has them positioned at $p_i = p(v_i)$. When we pass from these Cartesian coordinates to lattice coordinates q_i, we consider v_0 to be the origin, that is $q_0 = 0$, and then $\Lambda q_i = p_i - p_0$.

In this manner, the Cartesian description of the framework $\mathcal{F}$ given by $(p_0, ..., p_{n-1}) \in (\mathbb{R}^d)^n$ and $\Lambda \in GL(d)$, which requires $dn + d^2$ parameters, is reduced to $(q_1, ..., q_{n-1}, \omega)$, which involves only $d(n-1) + \binom{d+1}{2}$ parameters, since ω is a symmetric $d \times d$ matrix. The dimensional drop of $\binom{d+1}{2}$ reflects the factoring out of the action of the Euclidean group of isometries $E(d)$, which has this dimension.

We recall here the form of the equations expressing the constant (squared) length of edges, when using parameters $(q_1, ..., q_{n-1}, \omega)$ (cf. [7], formula (4.1)). Let us consider an edge (denoted here simply by e_{ij}) which goes from v_i to a vertex in the orbit of v_j. Then, in *Cartesian coordinates*, the edge vector is given by $p_j + \lambda_{ij} - p_i$, with some period $\lambda_{ij} = \Lambda n_{ij} \in \pi(\Gamma)$ and $n_{ij} \in \mathbb{Z}^d$. In *lattice coordinates*, the edge vector is given by $q_j + n_{ij} - q_i$ and the squared-length equation is:

$$\begin{aligned} \ell(e_{ij})^2 = \ & ||p_j + \lambda_{ij} - p_i||^2 = \\ = \langle \omega(q_j + n_{ij} - q_i), (q_j + n_{ij} - q_i) \rangle = \ & (q_j + n_{ij} - q_i)^t \omega (q_j + n_{ij} - q_i) \end{aligned} \quad (1)$$

This is the source of the linear system for computing infinitesimal deformations, as used in subsequent sections. Besides the elimination of equivalence under isometries, an obvious advantage of this formulation is that the Gram matrix $\omega = \Lambda^t \cdot \Lambda$ of the chosen basis of periodicity generators appears explicitly.

3. Auxetics and spectrahedra

We review now, following [9], the fundamental notions of geometric auxetics.

One-parameter periodic deformations. A *one-parameter deformation of the periodic framework* $\mathcal{F} = (G, \Gamma, p, \pi)$ is a smooth family of placements $p_\tau : V \to \mathbb{R}^d$, parametrized by time $\tau \in (-\epsilon, \epsilon)$ in a small neighborhood of the initial placement $p_0 = p$, which satisfies two conditions: (a) it maintains the lengths of all the edges $e \in E$, and (b) it maintains periodicity under Γ, via faithful representations $\pi_\tau : \Gamma \to \mathbf{T}(\mathbb{R}^d)$ which *may change with* τ *and give an associated variation of the periodicity lattice of translations* $\pi_\tau(\Gamma)$.

With our chosen generators for the periodicity group Γ, we have, at any moment of time $\tau \in (-\epsilon, \epsilon)$, a lattice basis Λ_τ and the corresponding Gram matrix $\omega_\tau = \omega(\tau) = \Lambda_\tau^t \Lambda_\tau$.

Auxetic path. A one-parameter deformation $(G, \Gamma, p_\tau, \pi_\tau), \tau \in (-\epsilon, \epsilon)$ is called an *auxetic path*, or simply *auxetic*, when the curve of Gram matrices $\omega(\tau)$ has all its tangents in the cone of positive semidefinite symmetric $d \times d$ matrices. When all tangents are in the positive definite cone, the deformation is called *strictly auxetic.*

When we operate in lattice coordinates $(q_1, ..., q_{n-1}, \omega)$, we use the abbreviations $\dot{q}_i = \frac{dq_i}{d\tau}(0)$ and $\dot{\omega} = \frac{d\omega}{d\tau}(0)$. From (1) we obtain the linear system for infinitesimal deformations $(\dot{q}_1, ..., \dot{q}_{n-1}, \dot{\omega})$:

$$\langle \dot{\omega} e_{ij}, e_{ij} \rangle + 2 \langle \omega e_{ij}, \dot{e}_{ij} \rangle = 0 \tag{2}$$

where $e_{ij} = q_j + n_{ij} - q_i$, with $n_{ij} \in \mathbb{Z}^d$, is meant to run over a complete set of representatives of edge orbits and $\dot{e}_{ij} = \dot{q}_j - \dot{q}_i$. For notational simplicity, the edge symbol e_{ij} omits the specific period shift, but it will be understood that several such edge representatives (with various shifts n_{ij}) may be implicated in the system. There are $d(n-1) + \binom{d+1}{2} = dn + \binom{d}{2}$ unknowns and $m = |E/\Gamma|$ equations.

Infinitesimally, our auxetic criterion requires $\dot{\omega}$ to be a positive semi-definite matrix, while strict infinitesimal auxeticity needs a positive definite $\dot{\omega}$. It follows immediately that *infinitesimal auxetic deformations* define a *cone* in the tangent space at $\mathcal{F}$ of the framework's deformation space. We speak of *infinitesimal auxetic capabilities* when there are infinitesimal deformations with $\dot{\omega} \neq 0$ and $\dot{\omega}$ positive semidefinite.

In convex optimization theory and semidefinite programming, an affine section of the positive semidefinite cone in the linear space of symmetric $d \times d$

matrices is called a *spectrahedron* [36, 30]. When the section goes through the origin we have a *spectrahedral cone*. Thus, when we look for infinitesimal auxetic capabilities, we have to look at the image of the space of infinitesimal deformations in the space of symmetric $d \times d$ matrices and examine its intersection with the positive semidefinite cone.

This important connection between infinitesimal auxetic capabilities of a periodic framework and semidefinite programming was established in [9], Corollary 7.1 and will be a pivotal element of the current investigation, which is targeted on a specific class of three-dimensional periodic frameworks with three degrees of freedom. From this perspective, our inquiry will be concerned with the six-dimensional vector space of 3×3 symmetric matrices and spectrahedral cones resulting from the intersection of the positive semidefinite cone with (generic) three-dimensional vector subspaces.

4. Regular three-dimensional periodic frameworks

There are several motivations for looking at three-dimensional periodic frameworks with three degrees of freedom. Applications to crystalline materials evidently require dimension three and important families studied for properties related to framework flexibility have, geometrically, three degrees of freedom. Zeolites, for instance, have framework structures made of vertex sharing tetrahedra and generic periodic frameworks of this type have, locally, a three-dimensional deformation space [4].

If we assume independent edge constraints in the linear system (2) obtained above for infinitesimal deformations, we see that a three dimensional solution space amounts to $m = 3n$. Mathematically, this type of periodic framework is quite relevant for periodicity relaxation problems, since this proportion of edge orbits to vertex orbits remains the same when adopting a sublattice of periods (of finite index).

As with similar definitions in rigidity theory, we have to assume certain genericity conditions on the framework, in particular independence of the edges [5]. For reasons that will become clear along the way, in this paper we consider only *regular periodic frameworks* in $\mathbb{R}^3$, defined by the following:

Conditions 1 (**Regularity conditions).**

i. The number of edge representatives is $m = 3n$.

ii. The edge constraints are independent, that is, the system (2) *has maximal rank* m.

iii. The projection from infinitesimal deformations to 3×3 *symmetric matrices:*

$$(\dot{q}_1, ..., \dot{q}_{n-1}, \dot{\omega}) \mapsto \dot{\omega}$$

is one-to-one.

iv. The projective cubic curve obtained by restricting the determinant function to the image of the above projection is non-singular.

We can now formulate precisely the problem solved in this paper:

Problem 2 (**Identify auxetic capability).** *Let* $\mathcal{F}$ *be a 3D* regular *periodic bar-and-joint framework. Decide if* $\mathcal{F}$ *allows strictly auxetic deformations.*

Remarks. Under the regularity conditions stated above, it follows from the implicit function theorem that the local deformation space of $\mathcal{F}$ is a *smooth threefold*. This means, in particular, that it is enough to solve the infinitesimal problem of *deciding if* $\mathcal{F}$ *has strictly auxetic infinitesimal deformations*, since any curve of symmetric matrices with a positive definite tangent direction at one point will maintain this property in a neighborhood of that point. In other words, $\mathcal{F}$ *allows strictly auxetic deformations* if and only if it *allows strictly auxetic infinitesimal deformations.*

Moreover, under the genericity condition (iv), intersecting the positive definite cone is equivalent with intersecting non-trivially its closure, the positive semidefinite cone, and we have a transversal intersection with the boundary in the generic case. Thus, our decision problem turns into the general question about infinitesimal auxetic capabilities which can be solved by semidefinite programming as stated in [9], Corollary 7.1. The solution presented in this

paper for our distinctive class of frameworks shows that geometric characteristics can be used for alternative algorithms, and thus avoid the general machinery of semidefinite programming [31].

5. Ternary cubic forms and their invariants

In this section we explain our geometrical approach, present the theoretical basis of the decision algorithm and review the classical results about elliptic curves.

We have shown above that the question about strictly auxetic deformations of a regular periodic framework $\mathcal{F}$ leads to an intersection problem in the space of 3×3 symmetric matrices between the positive semidefinite cone and a three-dimensional vector subspace image of the infinitesimal deformations of $\mathcal{F}$. Strictly auxetic deformations exist if and only if the three-dimensional vector subspace cuts through the positive definite cone.

Our approach is to investigate the resulting intersection with the boundary of the positive definite cone, which is contained in the vanishing locus of the determinant function. Since this function is a homogeneous cubic form, its restriction to our three-dimensional subspace gives a *ternary cubic form* and projectively, a real cubic curve in $P_2(\mathbb{R})$. The genericity condition (iv) allows the assumption that this cubic curve is non-singular (over the complex numbers $\mathbb{C}$).

Non-singular projective cubics are also known as *elliptic curves* and there is a wealth of classical results about them. We limit the main references to [3, 14, 35], which cover all the facts needed for our arguments. Different sources may have different choices of coefficients in front of certain invariants. Since we are concerned with real ternary cubics, we follow mostly [3].

We consider a three-dimensional real vector space with coordinates (x, y, z). We are interested in real cubic forms $f(x, y, z)$ and the projective cubic curves $f(x, y, z) = 0$ they define in $P_2(\mathbb{R})$, with projective coordinates $(x : y : z)$. There are ten distinct monomials of degree three in x, y, z and a ternary cubic form is determined by the ten coefficients of these monomials.

Hesse normal form. A non-singular real projective cubic $f(x, y, z) = 0$ is projectively equivalent over $\mathbb{R}$ with a unique cubic of the form:

$$x^3 + y^3 + z^3 - 3kxyz = 0 \tag{3}$$

with $k \in \mathbb{R},\ k \neq 1$. This form is called the Hesse normal form of the cubic. The three real inflection points are on the line $x + y + z = 0$, at $(0 : 1 : -1)$, $(-1 : 0 : 1)$ and $(1 : -1 : 0)$.

Aronhold invariants S and T. The action of the special linear group $SL(3)$ on the coordinates (x, y, z) induces a linear representation on the ten-dimensional vector space of ternary cubics. Homogeneous polynomials in the coefficients of ternary cubics are called invariant when they remain unchanged under this induced action. The Aronhold invariants S and T are given by two explicit invariant polynomials (with rational coefficients) of degree four, respectively six [35].

Discriminant. The discriminant Δ is the invariant polynomial of degree twelve given by:

$$\Delta = (4S)^3 + T^2 \tag{4}$$

A cubic form defines a non-singular curve in $P_2(\mathbb{C})$ if and only if $\Delta \neq 0$. For negative Δ, the real cubic in $P_2(\mathbb{R})$ is connected, while for positive Δ, it has two connected components.

Modular invariant J. For non-singular cubic forms, the *modular invariant* J is defined as a rational expression in the Aronhold invariants S and T by the formula:

$$J = \frac{(4S)^3}{(4S)^3 + T^2} \tag{5}$$

Since both numerator and denominator are homogeneous polynomials of degree twelve, the modular invariant J is invariant under the general linear group $GL(3)$. Moreover, two non-singular cubic curves in $P_2(\mathbb{C})$ are projectively equivalent over $\mathbb{C}$ if and only if J gives the same value when evaluated for the two cubic forms in the defining equations. This value is called the *modulus* of the curve.

For a cubic in *Hesse normal form* (3), we refer to the corresponding ternary form directly through the Hesse parameter k. Then, the values $S(k)$ and $T(k)$ are related to k by the following equations [14].

$$S(k) = -\frac{1}{2}k - \frac{1}{2^4}k^4 \tag{6}$$

$$T(k) = 1 + \frac{5}{2}k^3 - \frac{1}{2^3}k^6 \tag{7}$$

The discriminant takes the form:

$$\Delta(k) = (4S(k))^3 + T(k)^2 = (1 - k^3)^3 \tag{8}$$

and the case $k = 1$ in (3) is detected as singular.

For the modular invariant we find:

$$J(k) = \frac{(4S(k))^3}{(4S(k))^3 + T(k)^2} = \frac{k^3(k^3 + 8)^3}{64(k^3 - 1)^3} \tag{9}$$

and the right hand side is invariant under the involution $\eta(k) = \frac{k+2}{k-1}$. This means that $J(\eta(k)) = J(k)$, and the two curves are projectively equivalent over the complex numbers $\mathbb{C}$. The two fixed points of the involution η are $k_\pm = 1 \pm \sqrt{3}$ and $J(k_+) = J(k_-) = 1$. For *real Hesse cubics* i.e. $k \in \mathbb{R}, k \neq 1$, for any given real modulus there are exactly two real Hesse parameters with that modulus. The two curves *are not* projectively equivalent over $\mathbb{R}$, but as complex curves, they are projectively equivalent over $\mathbb{C}$. For more details and illustrations, we refer to [3].

For any non-singular cubic form f, we first compute the (values of) the Aronhold invariants $S(f)$ and $T(f)$ and then use formula (5) to compute the modulus $J(f)$. In the *real case*, we know that there is a *unique* real parameter k which gives a Hesse curve projectively equivalent over $\mathbb{R}$ with the curve $f = 0$, although, as reviewed above, there's another real parameter yielding the same modulus $J(f)$. The proper Hesse parameter k can be recognized as follows.

Lemma 1. *Let f be a non-singular ternary cubic form with Aronhold invariants $(S(f), T(f))$ and modulus $J(f)$. Then, the quartic equation in k^3 resulting from relation (9), namely:*

$$64J(f)(k^3 - 1)^3 = k^3(k^3 + 8)^3$$

has exactly two distinct real solutions, hence two distinct real solutions k_1 and k_2. If $T(f) \neq 0$, i.e. $J(f) \neq 1$, then $T(k_1)$ and $T(k_2)$ have opposite signs and the proper solution which gives a Hesse cubic projectively equivalent over $\mathbb{R}$ with the curve $f = 0$ must share the sign of $T(f)$. If $T(f) = 0$, then $S(k_1)$ and $S(k_2)$ have opposite signs and the proper solution must give the sign of $S(f)$.

Using (6), (7) and the action of the involution η, the Lemma follows from statements proven in [3]. After this brief review of relevant classical notions and results, we proceed with our inquiry. Let us observe first that, if our (generic) three-dimensional subspace of 3×3 symmetric matrices cuts through the positive definite cone, the corresponding (non-singular) real cubic curve must have *two connected components*. This follows from the fact that the intersection with the boundary of the positive definite cone gives one component which appears as a convex curve in adequately chosen affine planes. Since this component cannot contain inflection points, there must be a second component. We obtain:

Lemma 2. *If the discriminant of the ternary cubic f associated to the periodic framework $\mathcal{F}$ is negative, i.e. $\Delta(f) < 0$, then the framework does not allow non-trivial auxetic deformations.*

However, a positive discriminant is not a sufficient condition for strictly auxetic capabilities. We must check if the connected component without inflection points actually corresponds with positive semidefinite matrices. This can be determined by finding the explicit *real linear transformation* which takes the original cubic form to its Hesse normal form. Note that, by Proposition 1, the Hesse parameter can be determined from the invariants $(S(f), T(f), J(f))$. Then, the decision is *yes* if the preimage of $(1 : 1 : 1)$ corresponds to a positive or negative definite matrix and *no* otherwise.

We explain this procedure in more detail. For a cubic in Hesse normal form (3), the tangent lines at the three inflection points $(0 : 1 : -1)$, $(-1 : 0 : 1)$ and $(1 : -1 : 0)$ have equations $kx+y+z = 0$, $x+ky+z = 0$, respectively $x + y + kz = 0$. For non-singular real cubics (i.e. $k \neq 1$) these lines are concurrent only for $k = -2$, when the real curve is connected. Thus, for real cubics with two real components (i.e. $k > 1$), the three tangents and the line $x + y + z = 0$ of the inflection points give four points in general position in the dual projective plane $P_2(\mathbb{R})^*$.

It follows that, if we know the three real inflection points of a non-singular real cubic with two connected components, we can compute the three tangent lines and, after choosing a matching order for the inflection points, there is a unique real projective transformation which takes the line of real inflection points to the line $x+y+z = 0$ of the cubic's Hesse normal form and matches the inflection points and tangents. Obviously, this projective transformation

takes the cubic to its Hesse normal form. A different choice of matching order for the inflection points amount to composition with a permutation of the variables x, y, z.

An algorithm for computing the three real inflection points of a non-singular real cubic is described in [13].

For the Hesse form, the point $(1 : 1 : 1) \in P_2(\mathbb{R})$, as the only invariant point under permutations, must be in the interior of the triangle formed by the three tangents in the affine plane which has the line of inflection points at infinity. Since each connected component goes to itself under permutations, the component without inflection points must appear as a convex curve around the invariant point (and be contained in the triangle of tangents as well). Again, illustrations may be found in [3].

6. Decision algorithm for auxetic capabilities

A high level description of the algorithm is given below in Algorithm 1.

Input and Output. The input is a framework $\mathcal{F}$, with periodic graph $G = (V, E)$, $|V| = n$ and $|E| = 3n$, periodicity lattice given by the Gram matrix ω, and vertex representatives q_i presented in "lattice" or "crystallographic coordinates", as described in Section 2. In particular, q_0 is fixed at the origin, and each of the remaining $n-1$ points has 3 coordinates in the interval $[0, 1)$. In a pre-processing step we can check that the edges are independent, for example by writing the $3n \times 3n + 3$ rigidity matrix of the framework and computing its rank. The algorithm proceeds only if the rank is maximum. If the framework is not regular (cf. definition in Section 4), the algorithm will stop and report that it cannot give a precise answer. Otherwise, it reports the presence or not of auxetic capabilities. We remark that the algorithm runs on all *generic inputs*. In particular, the set of inputs on which it will stop without giving a definitive answer has measure zero.

Analysis. In Step 1, we set up the $3n$ linear equations (2) with $3n + 3$ unknowns $(\dot{q}_1, ..., \dot{q}_{n-1}, \dot{\omega})$ corresponding to the infinitesimal flexes $\dot{q}_i$ of the lattice coordinates $q_i, i = 1, \cdots, n-1$ of the framework and infinitesimal changes $\dot{\omega}$ in the 6 parameters describing the symmetric Gram matrix ω. We solve the linear system, and attempt to express $3n$ of the dependent variables in terms of 3 free variables chosen from among the $\dot{\omega}$. If this is not possible, then we stop and report that the framework is not regular. In Step 2, we

Algorithm 1 Decide existence of strictly auxetic deformations.

Precondition: $\mathcal{F}$ is a regular periodic framework.

function AUXETIC($\mathcal{F}$)

Step 1.

- Set up the linear system for periodic infinitesimal deformations.
- Solve it in terms of 3 independent variables chosen from the 6 giving the infinitesimal deformations of the Gram matrix.
- If this is not possible, STOP: the framework is not regular.

EndStep 1.

Step 2.

- $M \leftarrow$ Substitute the resulting linear forms in the 3×3 matrix of infinitesimal deformations of the Gram matrix.
- Compute the determinant $Det(M)$. The result is a cubic form $C(X, Y, Z)$ in 3 variables, called X, Y and Z.

EndStep 2.

Step 3.

- Compute the Aronhold invariants S and T for C(X,Y,Z).
- Using S and T, compute the discriminant D of C(X,Y,Z).
- If $D = 0$, cubic is singular. **return** "not regular".
- If $D < 0$, **return** NO: the framework does not have infinitesimal auxetic deformations.

EndStep 3.

Step 4.

If $D > 0$:

- compute the 3×3 linear matrix L for the transformation of the cubic $C(X, Y, Z)$ to the Hesse normal form $H(x, y, z)$.
- Compute the pre-image of the point $(1, 1, 1)$. This is a vector of specific values for (X, Y, Z).
- The corresponding constant symmetric matrix M is then tested for being definite (either positive or negative definite) and the corresponding output is produced:
- **return** YES, if definite or **return** NO, if indefinite.

EndStep 4.

end function

compute the determinant of the 3×3 infinitesimal Gram matrix $\dot{\omega}$, whose entries are linear forms in the three free variables and obtain the ternary cubic described in Section 5. In Step 3, we compute the S and T Aronhold invariants of the cubic and the discriminant Δ described in Section 5. We stop if $\Delta = 0$: the framework violates the regularity conditions. If $\Delta < 0$, the framework does not have auxetic capabilities, cf. Lemma 2. Otherwise, if $\Delta > 0$, we apply the procedure described in Section 5 after Lemma 2 to distinguish, correctly, the auxetic and non-auxetic cases.

Complexity. The running time of the algorithm is dominated by Step 1 (Gaussian elimination) and takes $O(n^3)$ arithmetic operations. The other steps are constant time calculations involving equations of degree at most 3.

Extensions. The decision algorithm can be easily modified to return an actual auxetic infinitesimal deformation. Indeed, the pre-image of the point $(1 : 1 : 1)$ in step 4 gives specific values for the free variables X, Y, Z of the cubic from Step 2, and all the infinitesimal deformation variables (for the points q and for the Gram matrix ω) can be expressed in terms of these three values, cf. Step 1. Finally, the step-by-step calculation of infinitesimal auxetic deformations can be used in a standard numerical simulation, with a sufficiently small time step, of an auxetic trajectory, if one exists.

7. Examples

We now illustrate our method with a type of structure as shown in Fig. 3. We define a family of periodic frameworks $\mathcal{F}(\lambda)$ in $\mathbb{R}^3$ with $n = 2$ vertex orbits and $m = 3n = 6$ edge orbits. The periodicity lattice is the standard integer lattice Z^3 and the chosen generators are the vectors $e_i, i = 1, 2, 3$ of the standard basis. The first orbit of vertices is represented by the origin (the red point in Fig. 3), and coincides with Z^3. For $\mathcal{F}(\lambda)$, the second orbit of vertices is represented by the point $p = p(\lambda) = \lambda(e_1 + e_2 + e_3)$ (the green point in Fig. 3). The edge orbits are represented by six edges connecting p with the vertices of the other orbit placed at $e_1, e_2, e_3, e_1 + e_2, e_2 + e_3, e_3 + e_1$ (the thick blue edges in Fig. 3).

In lattice coordinates (q, ω), the framework $\mathcal{F}(\lambda)$ will have $q = \lambda(e_1 + e_2 + e_3)$ and $\omega = I_3$, the identity matrix. Although $q = p$ in our initial setting, we maintain the notational distinction between lattice coordinates and Cartesian coordinates. Thus, the six edge vectors in lattice coordinates are written as $E_i = e_i - q,\ i = 1, 2, 3$ and $E_{jk} = e_j + e_k - q,\ ij \in \{12, 23, 13\}$,

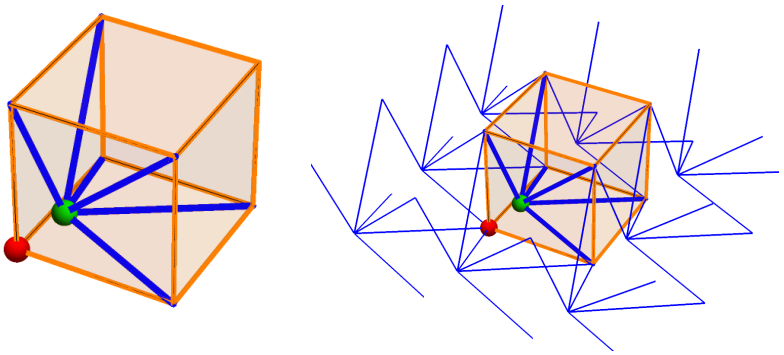

Figure 3: A 3D periodic framework with $n = 2$ vertex and $m = 3n = 6$ edge orbits. (Left) The unit cell with the 2 vertex representatives (colored) and the 6 edge representatives. (Right) A small $2 \times 2 \times 1$ fragment of the infinite framework.

and the linear system (2) for infinitesimal deformations takes the form:

$$\begin{aligned} \langle \dot{\omega} E_i, E_i \rangle - 2\langle E_i, \dot{q} \rangle = 0 \quad \text{for} \quad i = 1, 2, 3 \\ \langle \dot{\omega} E_{jk}, E_{jk} \rangle - 2\langle E_{jk}, \dot{q} \rangle = 0 \quad \text{for} \quad j, k = 1, 2, 3, j \neq k \end{aligned}$$

Exploiting permutation symmetry and choosing the diagonal elements of $\dot{\omega}$ as parameters, the three-dimensional space of solutions $\dot{\omega}$ is given by symmetric 3×3 matrices with equal off-diagonal entries of the form:

$$\dot{\omega}_{kl} = \frac{\lambda(1-\lambda)}{2 - 6\lambda(1-\lambda)} \cdot (\sum_{i=1}^{3} \dot{\omega}_{ii}) \tag{10}$$

We notice the invariance of the fractional coefficient in (10) under the involution $\lambda \mapsto 1 - \lambda$, which comes from the isomorphism of the frameworks $\mathcal{F}(\lambda)$ and $\mathcal{F}(1-\lambda)$ when reflecting in the plane $x_1 + x_2 + x_3 = 1/2$ (in Cartesian coordinates).

For simpler expressions, we introduce the following notations:

$$\ell = \lambda(1-\lambda), \quad \mu = \frac{\lambda(1-\lambda)}{2 - 6\lambda(1-\lambda)} = \frac{\ell}{2 - 6\ell}, \quad \rho = \mu^2(2\mu - 1) \tag{11}$$

We notice that, for $\lambda \in (-\infty, \infty)$, we have $\ell \in (-\infty, 1/4]$ and $\mu \in (-1/6, 1/2]$, with the resulting range $\rho \in [-1/27, 0]$.

We also rename our parameters as $X = \dot{\omega}_{11}$, $Y = \dot{\omega}_{22}$ and $Z = \dot{\omega}_{33}$. Then the cubic equation given by $det(\dot{\omega}) = 0$ becomes:

$$XYZ + \rho(X + Y + Z)^3 = 0 \tag{12}$$

It is easily verified that the points $(0 : 1 : -1)$, $(-1 : 0 : 1)$ and $(1 : -1 : 0)$ are inflection points of this cubic curve. The corresponding tangent lines are $X = 0$, $Y = 0$ and $Z = 0$.

The last part of the algorithm requires the computation of the real projective transformation which takes a given cubic form to the Hesse normal form:

$$x^3 + y^3 + z^3 - 3kxyz = 0. \tag{13}$$

In this case, it is easy to see that (up to permutation), the relation between (12) and (13) takes the form:

$$X = kx + y + z$$

$$Y = x + ky + z$$

$$Z = x + y + kz$$

with the parameters ρ and k related by:

$$\rho = -\frac{k^2 + k + 1}{3(k + 2)^3} \tag{14}$$

This formula follows from the necessary vanishing of monomial coefficients for x^2y etc. The singular case $k = 1$ for (13) corresponds with the singular case $\rho = -1/27$ for (12). The case $k = -2$ cannot arise, since $\rho = \pm\infty$ is excluded.

We remark that the point $(x : y : z) = (1 : 1 : 1)$ always corresponds with $(X : Y : Z) = (1 : 1 : 1)$. For $X = Y = Z = 1$ we have the symmetric matrix:

$$M(\mu) = \begin{pmatrix} 1 & 3\mu & 3\mu \\ 3\mu & 1 & 3\mu \\ 3\mu & 3\mu & 1 \end{pmatrix}, \quad \mu \in (-1/6, 1/2] \tag{15}$$

which is positive definite for $\mu \in (-1/6, 1/3)$ and indefinite for $\mu \in (1/3, 1/2]$.

We should remain aware of the fact that $\rho = 0$ and $\rho = -1/27$ in (12) give singular cubics, hence the framework $\mathcal{F}(\lambda)$ will be *non-regular* for $\lambda = 0, 1/3, 1/2, 2/3, 1$.

Particular cases. We consider the three cases $\lambda = 1/6, 1/3, 5/12$ and follow the algorithm.

For $\lambda = 1/6$, by STEP 3, we obtain the invariants:

$$S = -\frac{2287}{4000752},\ T = -\frac{2021723}{18525482136},\ \Delta = \frac{1000000}{22067482534159923}$$

In STEP 4 we find $k = 25.6407$ and, via (15), the output is *YES: the regular framework admits an auxetic deformation.*

For $\lambda = 1/3$, by STEP 3, we obtain the invariants:

$$S = -\frac{1}{11664},\ T = \frac{1}{157464},\ \Delta = 0$$

Since $\Delta = 0$ the algorithm stops with the message that *the framework is NOT REGULAR.*

For $\lambda = 5/12$, by STEP 3, we obtain the invariants:

$$S = -\frac{9973}{25625808},\ T = -\frac{45441143}{760048652376},\ \Delta = \frac{7353062500}{37144672966729275363}$$

In STEP 4 we find $k = 10.6042$ and, via (15), the final output is *NO: the regular framework does not admit an auxetic deformation.*

8. Algorithmic alternatives

It will be observed that the decision algorithm described in Section 6 gives more than just the recognition of strictly auxetic capabilities in the regular case. It provides, via the Hesse form, access to a normalized description of the spectrahedral cone of all auxetic infinitesimal deformations of the given framework. Information about variations of this cone as the framework deforms can be used for investigations of global aspects of auxetic behavior.

For the restricted purpose of a decision algorithm, we mention here two alternatives. The question about strictly auxetic capabilities can be approached with algorithms which produce sample points on all connected components of an affine real semi-algebraic set [1], sections 5 and 12. In our case, once we have our ternary cubic f, we ask for sample points on all connected components of $\{x \in \mathbb{R}^3 : f(x) > 0\}$ and then for sample points on all connected components of $\{x \in \mathbb{R}^3 : f(x) < 0\}$. Altogether, we have sample points on all connected components of the complement of $\{x \in \mathbb{R}^3 : f(x) = 0\}$. We then sweep the list of the corresponding 3×3 symmetric matrices, checking for definiteness, as in the final segment of Step 4 in our Algorithm 1. This approach does not need the assumption that f is non-singular.

The second alternative may answer the question about auxetic infinitesimal capabilities in a more general setting, but needs more refined genericity assumptions [21]. When applicable, it provides a smallest rank sample point on a given spectrahedron and, in our setting, would detect an auxetic infinitesimal deformation of the given framework.

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