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Introducing Spacial Graphs (updated version)

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Abstract

We introduce spatial graphs through a natural extension of the concept of planarity in three dimensions. For a graph G=(V,E), a face is a simple cycle of edges, and a complete set of faces is such that each edge belonging to a cycle in E is on at least one face in the set. G is spatial if admits a three-dimensional representation R with a complete set of faces consisting of simple surfaces, such that no two faces intersect except along the common edge. In particular G is called k-spatial if R includes k cells (spatial regions); and is called plane-face spatial if all the faces in R are plane. We prove that all graphs are 1-spatial, but not all of them are (k¿1)-spatial or plane-face spatial. In particular, K_n is $(n^2 - 3n)/2$-spatial and plane-face spatial. We derive some basic properties of spatial graphs as natural three-dimensional extensions of the properties of planar graphs.

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1 The concept of spatial graph

The discovery of Euler's theorem on polyhedra (1736) can be seen as the starting event in the theory of planar graphs, although other related results are certainly much older. Kuratowski's theorem (1930) was the second fundamental step in the field. Hopcroft and Tarjan's discovery of a linear time algorithm for testing planarity (1974), and Appel and Haken's proof of the four color theorem (1977), have brought the theory to the attention of theoretical computer scientists, while the relevance of planar graphs in many application areas has raised the interest of engineers and other scientists. An excellent comprehensive presentation of the whole subject can be found in [7].

As known, a planar graph $G = (V, E)$ can be drawn in a plane in such a way that no two edges intersect, except, possibly, in one of the extremes. Let G be non directed, simple (i.e., has no loops or multiple edges) and connected. And let v, e, f respectively denote $|V|$, $|E|$, and the number of faces in a plane representation of G (including the infinite face). The following well known results hold for planar graphs.

Facts 1 *a) (Euler).* $v - e + f = 2$.

b) $e \leq 3v - 6$, *for* $v \geq 3$.

c) There exists a vertex of degree (number of incident edges) ≤ 5.

d) (Kuratovski). A graph is planar iff it does not contain K_5, *or* $K_{3,3}$, *or a subdivision of these graphs.*

e) (Hopcroft and Tarjan). Planarity can be tested in O(v) time.

f) Every planar graph is 4-colorable, and can be 5-colored in O(v) time.

In this note we introduce *spatial graphs*, through a natural extension of the concept of planarity in three dimensions. In fact, a spatial graph admits a spatial representation where no two faces intersect. First we have to define a representation exactly. For a (non directed, simple and connected) graph $G = (V, E)$ we pose:

Definition 1 *a) A* **face** *of G is a simple cycle of edges (i.e., each vertex in the cycle is encountered exactly once). A* **complete set F** *of faces is such that each edge belonging to a cycle in E is on at least one face in F.*

b) A **representation R(G,F)** *of G with complete set F, is a three dimensional entity with vertices, edges and faces. Vertices and edges correspond to the elements of V and E, respectively. Faces are finite simple surfaces, each bounded by a cycle in F. (We speak of vertices, edges and faces as the elements of V, E and F, or their corresponding geometrical entities in the representation). R(G,F) is a* **valid representation** *if*

i) any two faces do not intersect (i.e., have points in common), except along the common edges, if any;

ii) if S is the union of all the faces in R(G,F), any closed line on S can be continuously shrunk to a single point, always remaining on S (i.e., S has no "holes").

c) A **cell** *of R(G,F) is a simple and connected spatial region wholly delimited by faces. All cells are finite except one (the infinite cell), and all delimited regions are cells (i.e., R(G,F) occupies the whole space).*

d) A valid representation R(G,F) is a **tree representation** *if has exactly one cell (in fact, the infinite cell).*

Note that the faces in $R(G,F)$ are bounded by at least three edges, and the finite cells are bounded by at least three faces. For example, consider the following graph G_1 with complete set of faces F:

$$G_1 = (\{a, b, c, d\}, \{ab, bc, cd, da, bd\}), \quad F = \{abcd, abd, bcd\}.$$

Each valid representation $R(G_1, F)$ has one finite and one infinite cell, both delimited by the three faces of F. Note that not all faces can be plane, otherwise they would intersect. If one of the faces is eliminated from F, $R(G_1, F)$ becomes a tree representation.

Definition 2 *A graph G is* **k-spatial***, with k integer ≥ 1, if there exists a valid representation of G with k cells.*

Note that spatiality requires the *existence* of a proper complete set of faces as a basis of a valid representation. The graph G_1 above is 2-spatial. However, it is immediate to note that not all graphs are $(k > 1)$-spatial. (For example, all graphs with at most two cycles of edges cannot have a finite cell). We also have:

Lemma 1 *a) All graphs are 1-spatial (i.e., admit a tree representation). b) Any k-spatial graph, with $(k > 1)$, is also $(k-1)$-spatial.*

Proof *For both points we show how to build a valid representation.*

a) By induction on v. Immediate for $v \leq 3$. For a generic graph G with v vertices, assume that a tree representation R exist. Consider the new graph H obtained by inserting in G a new vertex y, and new edges from y to an arbitrary subset X of vertices of G. There exists a tree $T \subseteq G$ containing all the vertices of X, such that all the leaves of T belong to X. The representation R can be continuously distorted in such a way that the vertices and edges of T lie on a plane P, and the rest of R lies on one side of P. Then, y is placed on the other side of P, and a surface from y to T

is built on this side without forming any closed cell. A tree representation for H then results.
b) In a valid representation with k cells, let A be a face separating two distinct cells C_1, C_2. Note that each edge of A must belong to at least another face, otherwise C_1 and C_2 would form a unique region. If A is removed, the set of faces remains complete and the representation remains valid. Clearly C_1 and C_2 are merged into a unique cell, hence k is decreased by 1.

A stronger definition of spatial graphs is perhaps more natural. It refers to a representation consisting of an aggregate of polyhedra.

Definition 3 *A graph G is* **plane-face spatial** *if is k-spatial for an arbitrary value k, and all the faces in the corresponding representation are plane. G is also called plane-face k-spatial.*

Note that the finite cells of the plane face representation of a plane-face spatial graph are bounded by at least four faces (tetrahedra). If we insist that all finite cells are polyhedra, the edges must be represented as straight-line segments, and any two faces bounding the same cell must lie on different planes. The graph

$$G_2 = (\{a, b, c, d, e\}, \{ab, bc, cd, da, de, eb\})$$

is plane-face spatial because admits the tree representation $R(G_2, F_2)$, with $F_2 = \{abcd, bcde\}$, and the two faces lying on the same plane. These faces have two common edges bc, cd, that need not be stright-line segments.

In lemma 1 we have proved that all graphs admit a tree-representation. This is no more true, if we pretend that all faces be plane. We have:

Lemma 2 *a) All complete graphs K_n are plane-face $\frac{n^2-5n+8}{2}$-spatial. b) Not all graphs are plane-face spatial.*
Proof *a) Immediate for $n = 2, 3$ ($n = 1$ is an uninteresting exception). For $n \geq 4$ we proceed by induction on n. For this purpose a "visibility" property is also inductively proved, namely, there exists a plane-face representation R for K_n, and a point y in its infinite cell, such that: (i) all the vertices $x_0, ..., x_{n-1}$ of K_n (taken in arbitrary order) are "visible" from y, and appear as vertices of a convex polygon P; (ii) the edges $(x_j, x_{(j+1) mod\, n})$, $j = 0, ..., n-1$, of K_n (also edges of P) are visible from y; (iii) the edges (x_{n-1}, x_j), $j = 1, ..., n-3$, of K_n (chords of P) are visible from y. P appears triangulated from y, and contains $n-2$ triangles all belonging to F_n. For $n = 4$, let F_4 be the set of all triangular cycles in the graph, and take a tetrahedron $R(K_4, F_4)$ as the basis for induction. Note that $R(K_4, F_4)$ has plane faces and $\frac{4^2-5\times4+8}{2} = 2$ cells, and the viewpoint y is easily found. For $n > 4$, the representation $R(K_n, F_n)$ is inductively obtained from the representation $R(K_{n-1}, F_{n-1})$ of the subgraph of K_n without vertex x_{n-1}. This vertex is placed in the infinite cell of $R(K_{n-1}, F_{n-1})$ such that it sees the vertices $x_0, ..., x_{n-2}$ of K_{n-1} along a convex polygon, and also sees the edges*

Figure 1: A representation of $K_{3,3}$. $\{a, b, c\}$ and $\{A, B, C\}$ are the two sets of independent vertices. The faces $aAbB, bBcC, cCaA$ form a complete set F, and may be placed on different planes. The representation can be distorted to have all straight-line edges.

$(x_j, x_{(j+1) mod\,(n-1)})$, $j = 0, ..., n-2$ and $(x_{n-2}, x_j), j = 1, ..., n-4$. Then, the new (plane) triangular faces $(x_{n-1}, x_j, x_{(j+1) mod\,(n-1)})$, $j = 0, ..., n-2$, and (x_{n-1}, x_{n-2}, x_j), $j = 1, ..., n-4$, are added to F_{n-1} to form F_n. This operation produces $n-3$ new tetrahedral cells, that is, the total number of finite cells of $R(K_n, F_n)$ is $(n-3) + (n-4) + ... + 1$. This value, increased by 1 for the infinite cell, sums up to $c = \frac{n^2-5n+8}{2}$.
b) We prove that $K_{3,3}$ is not p-spatial. $K_{3,3}$ has all faces of four or six vertices. Since $K_{3,3}$ is not planar (Kuratovski's theorem), the vertices cannot lie on the same plane, otherwise there would be two intersecting edges, hence two intersecting faces. Therefore, only faces with four vertices can be included in a complete set F, and no two faces F_1, F_2 of F can share three vertices, otherwise the five vertices in $F_1 \cup F_2$ would be on the same plane P, and the sixth vertex of $K_{3,3}$ should belong to another face F_3 which shares three vertices with $F_1 \cup F_2$, hence it should also belong to P. Since $K_{3,3}$ has nine edges, and each edge belongs to one or more cycles, at least three faces must occur in F, sharing two vertices pairwise. Without loss of generality, consider the set F shown in figure 1. If the three faces lie on different planes, the representation has a "hole", against definition 1.b.ii. Therefore an additional face must be included in F. Without loss of generality, let this face be $(aBcC)$, to be represented in a plane. Since this face shares three vertices with the face $(cCaA)$ of F, all six vertices must lie in the same plane.

In the following we refer to **spatial graphs**, meaning either k-spatial for some k, or p-spatial. We prove some basic properties of spatial graphs, and reinforce the definition of a graph by *assigning* the set of faces to it. We then discuss the relations between spatial graphs and other structures, and outline possible applications and some major open problems.

2 Basic properties of spatial graphs

For a valid representation $R(G, F)$ of a spatial graph, let f and c respectively denote $|F|$ and the number of cells (including the infinite cell). We have the following immediate extension of Euler's theorem:

Theorem 1 *Any valid representation of a spatial graph satisfies:*

$$v - e + f - c = 0. \tag{1}$$

Proof. *Let S be the union of all the faces in a valid representation $R(G, F)$. 1) If S contains faces which do not belong to the boundary of a finite cell, cancel these faces together with the vertices and edges not belonging also to the remaining faces. It can be immediately verified that the values of v, e and f change in such a way that relation 1 still holds. 2) Cancel one of the remaining faces. The values of f and c decrease by 1, and relation 1 still holds. 3) Repeat steps 1 and 2 until S is composed of one face. We now have $e = v$, $f = 1$ and $c = 1$, and relation 1 holds.*

The above proof technique is standard. Relation 1 is formally identical to the one of Poincaré extension of Euler's theorem to n-dimensional polyhedra [1]. Note, however, that the two extensions apply to different classes of figures. For example, graph G_1 of section 1 has a valid representation with three faces bounding one finite cell. This cell is not a polyhedron, still theorem 1 holds.

For a tree-representation of a spatial graph ($c = 1$), we have from theorem 1:

$$f = e - v + 1. \tag{2}$$

Relation 2 can be seen as the extension to $\mathbf{R}^3$ of the relation $e = v - 1$ holding for ordinary trees. We now pose two natural conditions on graph G, and its selected complete set of faces F. Namely:

Condition 1 *$e > v$ (hence $f \geq 2$ in any complete set of faces).*

Condition 2 *For any vertex x, each pair of incident edges yx, zx belong to at most one face of F.*

For example, graph G_1 satisfies condition 1, but its set F with three faces does not satisfy condition 2. We have:

Theorem 2 *In any valid representation of a spatial graph G obeying conditions 1 and 2 we have:*

$$f \leq 2(e - v). \tag{3}$$

Proof *1) First consider a vertex x of degree one, that is incident to exactly one edge xy. Remove x and xy from G, and iterate the process until no vertex of degree one remains. This does not alter the two sides of relation 3.*
2) Now consider a vertex x of degree two, incident to xy, xz. Note that, after step 1, xy and xz must belong to a cycle, and that condition 2 imposes that they belong to exactly one face F_1. Remove x, xy, xz and F_1. The left-hand side of relation 3 decreases by one, and the right-hand side decreases by two. Iterate steps 1 and 2 until a new graph

G' is obtained, with all vertices of degree ≥ 3. If relation 3 is valid for G', then a fortiori is valid for G, for which the left-hand side has been decreased no more than the right-hand side.
3) We prove relation 3 for G'. Consider the bipartite graph H with vertices corresponding to the elements of V and F, and an edge xz whenever a vertex $x \in V$ lies on face $z \in F$. Let h be the number of the edges of H. Each face contains at least three vertices, hence we have $3f \leq h$. For any vertex $x_i \in V$, $1 \leq i \leq v$, let $y_1x_i, ..., y_{k_i}x_i \in E$ be the edges incident to x_i in G'. There are at most $k_i(k_i-1)/2$ faces in F containing x_i, however, at most $3k_i - 6$ faces do not intersect other than in x_i or along an edge y_jx_i. In fact, the intersections of these faces with a small sphere centered in x_i must be non intersecting segments, whose endpoints are the intersections of the edges $y_1x_i, ..., y_{k_i}x_i$ with the sphere. This gives rise to a planar graph on the sphere, that must obey fact 1.b. Therefore we have $3f \leq h \leq \sum_{i=1}^{v}(3k_i - 6)$. Relation 3 easily follows, noting that $\sum_{i=1}^{v} k_i = 2e$.

Theorem 2 can be seen as an extension of fact 1.b to the subfamily of spatial graphs fulfilling conditions 1 and 2. For example K_5 has $v = 5$, $e = 10$, and $\binom{5}{3} = 10$ possible triangular faces. Since these values fulfill relation 3, it is conceivable that K_5 has a valid representation that includes all these faces (this is indeed true, see next corollary 3).

From theorem 2 we can also derive the following corollary whose proof is omitted for brevity. The result can be seen as an extension to $\mathbf{R}^3$ of fact 1.c.

Corollary 1 *In any valid representation of a spatial graph obeying conditions 1 and 2 there exists an edge with "face degree" (number of incident faces) $\leq 2m - 1$, where m is the maximum "edge degree" (number of edges) of a face.*

For example, if F includes only triangular faces, $R(G, F)$ must contain an edge belonging to at most five faces.

We have already noted that not all graphs are $(k > 1)$-spatial, but all are 1-spatial (lemma 1). For an arbitrary graph G we then pose:

Definition 4 *The* **spatiality degree** *$s(G)$ of G is the maximum value k for which G is k-spatial.*

The following corollary is an immediate consequence of theorems 1 and 2.

Corollary 2 *Under conditions 1 and 2 we have:*

$$s(G) \leq e - v. \tag{4}$$

For example K_6 contains $\binom{6}{4} = 15$ possible tetrahedra, but at most 8 of them may occur in a valid representation (we have $s(G) \leq e - v = 9$, and we must count the infinite cell in this number). This is indeed possible. We have:

Theorem 3 *For $n \geq 4$ all complete graphs K_n are $\frac{n^2-3n}{2}$-spatial, and fulfill relation 4 with equality.*

Proof *By a refinement of the argument used in the proof of lemma 2.a. In addition to points (i), (ii), (iii), the visibility property has a fourth point (iv), namely, there exists a point z in the infinite cell of R, such that the edges of P, and the chords (x_0, x_j), $j = 2, ..., n-2$, of P, are visible from z. That is, y and z are on "opposite sides" of P. Note that the inductive construction of $R(K_n, F_n)$ given in lemma 2 preserves also point (iv). For $n = 4$, take a tetrahedron $R(K_4, F_4)$. We have $\frac{4^2-3\times 4}{2} = 2$, and $e - v = 2$. For $n > 4$, build $R(K_n, F_n)$ as in lemma 2, then add to F_n the non-plane triangular faces (x_{n-1}, x_0, x_j), $j = 2, ..., n-3$. This operation produces $n-4$ new cells, that is, the total number of cells becomes $\frac{n^2-5n+8}{2} + n - 4 = \frac{n^2-3n}{2}$. We also have $e - v = \frac{n(n-1)}{2} - n = \frac{n^2-3n}{2}$, that is, relation 4 is fulfilled with equality.*

After having defined a valid representation of G as one based on the *existence* of a suitable set F of faces, we reinforce the definition of graph by adding the *specification* of F.

Definition 5 *An* **F-graph** *H=(V,E,F) is a graph with a specified complete set F of faces.*

In any representation of H the faces are therefore fixed. As it may be expected, not all F-graphs are spatial (that is, there is no value $k \geq 1$ for which they are k-spatial). Let FK_n denote the complete graph of n vertices, with F consisting of all the possible triangular faces. We have:

Corollary 3 *FK_n is spatial for $n \leq 5$, and is non spatial for $n \geq 6$.*

Proof *Immediate for $n \leq 4$. For $n = 5$ use the construction shown in the proof of theorem 3. For $n \geq 6$, FK_n has $f = \binom{n}{3}$, $e = n(n-1)/2$, and fulfills the hypotheses of theorem 2. We then have $\binom{n}{3} \leq 2(e-n) = n^2 - 3n$, impossible for $n \geq 6$.*

3 Spatial graphs and other known structures

We have stated that spatial graphs introduce a natural extention of planarity in three dimensions. A similar statement was made in [6], in connection with the definition of a *good embedding* of a graph G in $\mathbf{R}^3$. The main difference between the two approaches is that in [6] *all* the possible faces (cycles) of G are inserted in the representation, and two faces are allowed to intersect along a curve S whose endpoints are vertices of G, but is not required that S be composed of edges of G. This abundance of faces introduces a severe limit to the number of graphs which have a good embedding. Not surprisingly, complete graphs do not have one. Our approach, instead, is based on the existence of a suitable subset of cycles over which a valid representation can be built. This leads to much more flexible conditions, and to completely different results. We have also introduced F-graphs, where an arbitrary set of faces (not all possible faces) is assigned.

The existence of a valid representation for graphs or F-graphs seems to constitute a legitimate extension of planarity in $\mathbf{R}^3$.

Several areas have faced spaciality problems. In the field of solid modeling, polyhedral structures have been assigned as graphs, with the additional specification of a set of faces. The *integrity* of the model requires that the faces do not intersect [4]. In principle this integrity is assumed for the original object, and must be maintained under different transformations such us rotation, zooming, continuous deformations etc. This may cause major problems, due to precision and rounding of numerical calculations, or to degeneracy of the original inputs [5]. A comprehensive review of problems in solid modeling, related to the visualization of three dimensional objects, can be found in [2]. Although there is a gap still to be filled between theory and practice, we think that spatial graphs (in particular, plane-face spatial graphs) may be a useful tool in this area.

Another field where plane-face spatial graphs may constitute a relevant mathematical model is the one of crystallography. Here the vertices are arranged in regular lattices, and indicate positions of atoms, and any plane passing through lattice nodes contains a potential face of the crystal [8]. Hence there are infinitely many potential faces, although the probability that one such face actually appears in the external surface may be very little. The crystal is generally viewed as an aggregate of space-filling polyhedra, where the most probable faces are put into evidence. The existence of other representations seems to follow the rules of plane-face spatiality.

An area of particular importance, where the concept and properties of spaciality might be useful, is the one of protein structure [9]. Several other applications may also benefit from this theory, as the ones studied in [3]. In general, the relevance of spatial graphs in different areas, particularly in Engineering and Biology, must still be understood.

More than that, to set up a significant theory of spatial graphs the theoretical results of section 2 should be strengthened, and efficient algorithms for the new family of graphs should be developed. As challenging and urgent open problems let us mention the following.

1) Find an equivalent of Kuratowski's theorem to characterize spatiality of graphs ($K_{3,3}$ and FK_6 are natural candidates as forbidden patterns for plane-face graphs and F-graphs, respectively).

2) Devise an efficient algorithm to test if a graph is k-spatial for a given k, or to determine the spatiality degree of the graph.

3) Determine bounds on coloring and devise a face-coloring algorithm (corollary 1 is a possible basic tool).

4) Propose a good way of drawing spatial graphs, and devise an efficient embedding algorithm.

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