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# Deformational covariance of graphs

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Graphs on $n$ vertices are classified into equivalence classes under the linear group $L(n)$. All graphs representing the same operator on a vector space $V_n$ belong to the same class. Graphs of different operators may or may not belong to the same class as ascertained by rules that were given by the author. Graphs in the same class are "structurally covariant". If, in addition, two graphs can be continuously deformed into each other in the sense of varying line strengths while remaining structurally covariant throughout, then the two graphs are termed "deformationally covariant" along such paths. Applications in the quantum theory of chemistry and to the dynamic stability theory of coupled reaction systems which occur in various fields are indicated.

**Key words:** Deformations of graphs—molecular deformations

In a previous paper [1], a correspondence was established between algebraic structures built on a vector space $V_n$ and graphs of several kinds. In particular the space containing the linear operators $\{Q\}$ on $V_n$ is associated with a collection of graphs, directed graphs for arbitrary linear operators, non-directed ones with Hermitian operators. By "graph" we shall mean below the non-directed ones. Graphs may contain loops. Multi-graphs which would have multiple lines between a pair of vertices are not needed for our purpose here since each line may be assigned a "strength", commonly a + or − real number (in general could be complex too) corresponding to the algebraic sum of multilines between that vertex pair. Vertices represent vectors or their duals of $V_n$ or $V_n^+$ or the kets or bras of Dirac, etc. depending on the application intended.

The set of graphs $\{G_Q\}$ on $V_n$, on $n$ vertices, and $\{Q\}$, form a complete bilinear vector space (or a dyad space) if the strengths $\{q\}$ of the lines of $G$, taken here to be in the real field $\mathcal{R}$, are arbitrary. If however, there is a relation between the

vertices of $G$ and the points of the Euclidean 3-space, $\varepsilon_3$, then the statement is true only for $n \leq 4$. For $n > 4$, the $\{q\}$ have constraints due to distance geometry in $\varepsilon_3$. Such is the case for example in application to molecular structures and/or their quantum theory. In the embedded case [2] in the geometric sense, the $\{G\}$ do not form a complete vector space, nor a dyad space, but the $\{G\}$ can be classified [1, 3] into equivalence classes under the linear group $L(n, \mathscr{R})$.

Two $G$'s which are in the same $L$-equivalence class (i.e. $G_1 \overset{L}{=} G_2$) thereby called "structurally covariant [1]", can be obtained from each other by simple graph manipulations using two "star" and two "loop" rules given earlier [1].

If $\{\{G\}: G_1 \overset{L}{=} G_2 \cdots \overset{L}{=} G_k\}$, then they also have the same eigenvalue indices, the LPI, $\{n_+, n_0, n_-\}$, the numbers of +, 0, and − eigenvalues (for $G_Q \to Q$ with $Q = Q^+$ which is always the case if $G_Q$ is non-directed).

Take now two graphs $G_1$, $G_2$ on $V_n$, both of $n$-vertices, such that some lines are missing $\{q = 0\}$ in $G_2$ that are in $G_1\{q \neq 0;$ + or $-\}$.

We may have $G_1 \overset{L}{=} G_2$ or $G_1 \overset{L}{\neq} G_2$ as may be ascertained by the star-loop rules [1]. Suppose $G_1 \overset{L}{=} G_2$. We then ask the question, whether $G_1$ can be continuously deformed (either in the geometric sense if $\varepsilon_3$-embedded [2], or in the general case of arbitrary line strengths) such that the lines missing in $G_2$ become zero gradually while all the intermediate $G$'s, $\{\bar{G}\}$, remain $G_1 \overset{L}{=} \bar{G} \overset{L}{=} \bar{G}' \cdots \overset{L}{=} G_2$. The present paper deals with this question of "deformational covariance".

*Example of structurally covariant but deformationally not covariant graphs* $(=^{SC}, \neq^{DC})$ *and of both* $(=^{SC})$ *and* $(=^{DC})$ *cases.* Take an $n = 4$ $G$, Fig. (1), with its line strengths all equal (say $q = 1$).

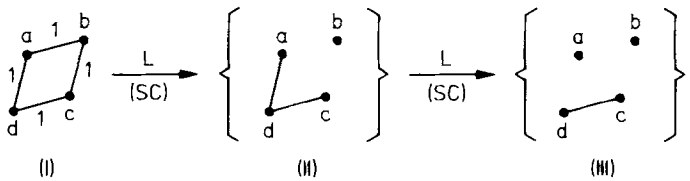


Fig. 1

By the star-rules [1], if in (I) vertex $d$ is multiplied by $(-1)$, then taken over to $b$, two lines get elimintated. Multiplying then $c$ with $(-1)$ and moving it onto $a$, the last graph in Eq. (1) results, which by the way also shows that $n_0 = 2$, $n_+ = n_- = 1$ for the initial $G$. The three $G$'s in Fig. (1) are structurally covariant.

What about now trying to get from graph-I to II, then to III not by the star rules but by stretching out some of the lines till they break? Will the LPI remain the same in the process? We can easily see that the answer depends on the type of deformation.

If we stretch out $b$ so that $q_{ab}$ and $q_{bc}$ remain equal to each other throughout, the LPI is preserved, and $G_I =^{DC} G_{II}$ along this path. (*Proof*: multiply $d$ by $\kappa = -q_{ab}$ at any value of $q_{ab}$, then take it onto $b$).

If on the other hand, we attempt to stretch only the $(ab)$ first, then $(bc)$, the LPI goes from $\{n_0 = 2,\ n_+ = n_- = 1\}$ to $\{n_+ = 2,\ n_- = 2\}$ initially. Such a path therefore does not lead to deformational covariance, even though the end graph $=^{SC}$.

Thus in comparing two graphs some deformation paths from one to the other continuously preserve linear covariance [4], some may not. The $G_1 =^{DC} G_2$ along the former paths.

*Theorem of deformational covariance*: Given some graphs $G_1, G_2, \ldots$ on $V_n$ with some of their lines differing in their strengths from graph to graph (including cuts, $q = 0$), if throughout continuous variations of those strengths (along some paths or modes), the graphs and their intermediates remain structurally covariant, then $G_1, G_2, \ldots$ are deformationally covariant (along those paths or modes). To ascertain deformational covariance $(\Rightarrow^{DC})_p$, the star-loop rules [1] are applied for continuously varying strength values (for each mode possible).

Proof is immediate from $=^{SC}$ theorems [1] applied at each value of each varying line strength (including at the $q = 0$ points where e.g. $q$ goes from $-$ to $+$).

*Applications*: *a*) In the quantum theory of chemistry and in structural chemistry, structural electronic diagrams for a given set of atoms differing in some lines correspond to isomers. Deformational covariance along some paths means there will not be much activation energy required, qualitatively speaking, along such "reaction paths". This principle [1–4] is considerably more general than the usual use of only the point group symmetries (cf. Refs. given in Ref. 1 and Ref. 3 of this paper) where they exist.

*b*) Molecular orbital theories [5] involve one and two center interaction parameters in their Hamiltonians. The present theory allows one to find out whether any qualitative conclusions from such methods would change as parameters are varied.

*c*) Dynamical stability [6] of coupled reaction systems whether in chemistry, ecology, or economics, may be treated by certain networks which are graphs of two kinds of lines and two kinds of vertices [7]. The "rate constants" of elementary reaction steps in these may be associated with "strengths" of one kind of line. Then, how the qualitative dynamics and stability behavior (even in the non-linear cases which are common there) are affected within regions of the parameter ("rate constant") space, can be ascertained by the methods of the present theory [1–4, 7].

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