Graph equivalence and characterization via a continuous evolution of a physical analog

Vladimir Gudkov\textsuperscript{1,} and Shmuel Nussinov\textsuperscript{2,} \\
\textsuperscript{1}Department of Physics and Astronomy \hfill \textsuperscript{2}Tel-Aviv University \hfill University of South Carolina Columbia, SC 29208 \hfill School of Physics and Astronomy \hfill Tel-Aviv, Israel \hfill and \hfill Department of Physics and Astronomy \hfill University of South Carolina Columbia, SC 29208 \hfill (Dated: February 1, 2008) \\

Abstract \\

A general novel approach mapping discrete, combinatorial, graph-theoretic problems onto “physical” models - namely \(n\) simplexes in \(n-1\) dimensions - is applied to the graph equivalence problem. It is shown to solve this long standing problem in polynomial, short, time.
INTRODUCTION

A graph G consists of n vertices \( V_i \) connected by edges \( E_{ij} \). It is described by a connectivity matrix \( C \) with:

\[
C_{ij} = C_{ji} = 0, 1 \quad \text{(for (dis)connected } V_i \text{ and } V_j \text{ i} \neq j = 1, \cdots, n) \]

\[
C_{ii} = 0 \quad (1)
\]

Vertex relabelling \( i \rightarrow p(i) \) leaves G invariant but changes C according to

\[
C \rightarrow C' = P^T C P \quad (2)
\]

with \( P \) an orthogonal matrix with only one non-zero element in each row \( i \) and column \( j = p(i) \), which represents the above permutation

\[
P = \delta_{(j,p(i))} \quad (3)
\]

The graph equivalence problem is the following: “Given \( C \) and \( C' \), how can we decide, in time which is polynomial in \( n \), if both correspond to the same topological graph \( G \) or to different graphs?, or stated differently, does a permutation matrix \( P \) for which Eq.(2) holds exist, and what is this \( P \) matrix?”

Exhaustive testing of all \( n! \) permutation is impractical even for moderate \( n \). A more systematic search of \( P \) performs just those transpositions which enhance an “overlap” function say

\[
trC'TC' = \sum_{ij} C_{ij}C'_{ij} \quad (4)
\]

However the changes in \( C \) (and in \( trC'TC' \)) due to any permutation is finite. There is no algorithm for systematically enhancing \( trC'TC' \), as subsequent transpositions may undo the improvement due to previous permutations.

Our basic suggestion is: Instead of using discrete, large changes of say just two elements in a transposition \( (i \leftrightarrow j) \), we modify, in each step, all elements by small amounts.

Such “continuous” changes seem impossible: in the strict formal approach there are no “continuous permutations”.
THE DYNAMICAL MODEL FOR SIMPLEX DISTORTION

We use a symmetric \( n \) simplex (in \( n - 1 \) dimensions) to represent our graph. The “abstract” vertices \( V_i \) of \( G \) (or \( C \)) are mapped into the geometrical vertices \( \vec{r}_i \), \( i = 1, \ldots, n \) of the simplex. The symmetric configuration with all \( |\vec{r}_i - \vec{r}_j| \quad i \neq j = 1, \ldots, n \), equal, is the starting point of our algorithms.

The motion generated by the dynamics, was designed to distort the simplex by shifting its vertices from the symmetric initial positions. The distorted simplex then reveals characteristic features of the graph \( G \).\[1\]

The original aim of the distortion algorithm was to find groups of vertices in \( G \) with higher than average mutual connectivity, and assess the distances between the various clusters in the graph.

To this end attractive (repulsive) interactions were introduced between fictitious point objects at \( \vec{r}_i \) and \( \vec{r}_j \) when the corresponding vertices \( V_i \) and \( V_j \) are connected (or disconnected) in \( G \). We use first order “Aristotelian” dynamics:

\[
\mu \frac{d\vec{r}_i(t)}{dt} = \vec{F}_i(\vec{r}_i(t)),
\]

(5)

with forces \( \vec{F}_i \) which derive from potentials:

\[
\vec{F}_i = -\nabla_{(\vec{r}_i)} \{ U[\vec{r}_i, \ldots, \vec{r}_n] \},
\]

(6)

\[
U = \sum_{i>j} U_a(|\vec{r}_i - \vec{r}_j|)C_{ij} + \sum_{i>j} U_r(|\vec{r}_i - \vec{r}_j|)(1 - C_{ij}),
\]

(7)

\( U_a(r) \) (\( U_r(r) \)) are attractive (repulsive) pair-wise potentials.

By a proper tuning of the latter- which can even be modified as a function of “time” - we can physically cluster at separate locations groups of points representing strongly (internally) connected clusters in the graph \( G \).

To avoid collapse towards the origin (or a “run-away” to infinity) if \( U_a \) (or \( U_r \)) dominates, we force \( \vec{r}_i(t) \) to stay, at all times, on the unit sphere:

\[
|\vec{r}_i(t)| = 1 \quad \text{all} \quad t > 0.
\]

(8)

The graph characterization (G.C.) and graph equivalence (G.E.P.) problems are very closely connected. If we could find (in polynomial number of steps!) a set of real numbers \( \rho_1, \rho_2, \ldots, \rho_m \) that would completely characterize a graph \( G \) then the G.E.P is readily solved.
All we need to do is to compute for $C$ ($C'$) these numbers $\{\rho_k\}$ ($\{\rho_k'\}$), order the $\rho_k$ and $\rho_k'$ sets separately and compare them.

The set of eigenvalues ($\lambda_1, \cdots, \lambda_n$) of the connectivity matrix are certainly invariant under relabelling. While this set encodes a rich body of information of graph theoretic interest, it fails to completely characterize graphs\cite{4}.

An alternative and natural simple variable helping characterize connectivity matrices is the mutual entropy (see, for example \cite{3}). Suppose the connectivity matrix $C$ has been normalized so that

$$\sum_{i,j=1}^{n} C_{ij} = 1. \quad (9)$$

$P_i = \sum_j^n C_{ij}$ could then be considered as the probability that $V_i$ and $V_j$ are connected. The corresponding entropy

$$H(\text{row}) = -\sum_{j=1}^{n} P_i \log P_i, \quad (10)$$

could be considered as a measure of the uncertainty of the rows connection for the given network. The amount of uncertainty for the connection of the column nodes given that the row nodes are connected is

$$H(\text{column}|\text{row}) = -\sum_{i,j} C_{ij} \log C_{ij} - H(\text{row}). \quad (11)$$

As a result the amount of $\text{mutual information}$ gained via the given connectivity of the network is

$$I(C) = H(\text{row}) + H(\text{column}) - H(\text{column}|\text{row}), = \sum_{i,j} C_{ij} \log (C_{ij}/P_iP_j). \quad (12)$$

where

$$H(\text{column}|\text{row}) = -\sum_{i,j} C_{ij} \log (C_{ij}). \quad (13)$$

Due to the double summation and the symmetry of the connectivity matrix $I(C)$ does not depend on the vertex relabelling and is a permutation invariant measure for the connectivity matrix.

Calculations of the mutual entropy for two connectivity matrices provides an easy way to distinguish between these corresponding different graphs. If, however, the entropies are the same, the more detailed approach below is used. Amusingly we found that the entropy is already sufficient to distinguish between the lowest cospectral graphs (see, for example \cite{4} and references therein).
The distances between the various vertices
\[ r_{ij}(t) \equiv |\vec{r}_i(t) - \vec{r}_j(t)| \] (14)

vary in our original algorithm as a function of time away from the original common value:
\[ r_{ij}(0) = |\vec{r}_i(0) - \vec{r}_j(0)| = a \quad \text{all } i \neq j = 1, \ldots, n \] (15)

Also in identical simulations of the dynamical evolution, the sets of relative distances computed for \( C \) and \( C' \), should be the same if \( C \) and \( C' \) are equivalent:
\[ \{r_{ij}(t)\} = \{r'_{ij}(t)\} \] (16)

One permutation of \( n \) elements (namely that which brings via Eqs.(2) and (3) \( C \) into \( C' \)) should yield:
\[ |\vec{r}_{p(i)}(t) - \vec{r}_{p(j)}(t)| = |\vec{r}'_{i}(t) - \vec{r}'_{j}(t)| \] (17)

It is straightforward to verify (16) and then using (17) recover the permutation \( i \rightarrow p(i) \).

In essence the idea of the present algorithm is to use the distortion of the simplex \( S(0) \rightarrow S(t) \) \{i.e. \( \vec{r}_i(0) \rightarrow \vec{r}_i(t) \)\} generated via the dynamics of (repulsion) attraction between (dis)connected vertices in \( G \) to bring out an “intrinsic shape” of the graph.

Initially all vertices were at equal distances\[5\]. All the information pertaining to the graph was encoded in the interactions of Eq.(7).

After enough evolution steps, each vertex moves appreciably away, namely by
\[ |\vec{r}_i(t) - \vec{r}_i(0)| \approx a/2 \] (18)

from its initial position. The information on the specific graph \( G \) reflects in the geometrical shape of \( S \), i.e. the set of distances,
\[ |\vec{r}_i(t) - \vec{r}_j(t)| \quad i \neq j = 1, \ldots, n. \] (19)

Vertices which are near in a graph theoretic sense, namely for which there are many, short, connecting paths in the graph move closer together. (A short path consists of a small \# of consecutive edges which starts at \( V_i \) say and terminates at \( V_j \)). Like wise vertices which are
far in a graph theoretic sense i.e. have fewer and longer connecting paths will tend to move further away.

In our earlier work[6] we sought to identify “clusters in the graphs” namely have the points corresponding to a subset \{C_i\} of vertices in the graph which have relatively strong mutual, internal, connectivity, collapse to a single point.

For the present purpose we need (and should!) not pursue the evolution that far, as by then the graph simplifies and some of the inter-cluster details are lost. Rather we need to stop “Half-Way”: after Eq.(19) holds and yet no cluster has completely collapsed.

Note that in \(n-1\) dimensions all the \(n(n-1)/2\) distances \(|\vec{r}_i(t) - \vec{r}_j(t)|\) are independent, apart from triangular inequalities of the form

\[
|\vec{r}_i(t) - \vec{r}_j(t)| \leq |\vec{r}_i(t) - \vec{r}_k(t)| + |\vec{r}_k(t) - \vec{r}_i(t)|.
\]  

(20)

Jointly these distances specify the geometric shape of \(S\).

The mapping of the \(n(n-1)/2\) bits of information: \(C_{ij} = 0\ or\ 1\), via our dynamic evolution, into the set of \(n(n-1)/2\) distances, is highly non-linear. The fact that we have \(n(n-1)/2\) distances (rather than just \(n\) eigenvalues) makes the former more likely to specify the graphs.

Further we note that the time \(t\) when the comparisons are made and the attractive and repulsive interactions in Eq.(7) above are free parameters and functions. Hence we can repeat the above graph comparisons for many values and/or many functions \(U_r(\rho), U_a(\rho)\), making the significance of a successful match extremely high.

If many of the \(r_{ij}(t)\) \{and \(r'_{ij}(t)\)\} are degenerate our ability to resolve graphs will be diminished. However such degeneracies must stem from some symmetries in the graphs and corresponding connectivity matrices. Once these symmetries are identified, the number of independent \(C_{ij}\) \(or\ C'_{ij}\) and the task of comparing them will be accordingly reduced.

We apply the above approach below, demonstrating its power and versatility.
THE CONVERGENCE AND COMPLEXITY OF THE DISCRETE MODELINGS OF THE DYNAMICAL EVOLUTIONS

We follow the dynamics of the vertex shifts in Eq.(5) by discretizing the first order equations:

$$\vec{r}_i(t + \delta) = \vec{r}_i(t) + \frac{\delta}{\mu} \vec{F}_i(\vec{r}_i(t)) \tag{21}$$

with $\delta$ a small time increment.

Since $\vec{r}_i, \vec{F}_i$, are $n-1$ dimensional vectors Eq. (21) represents $O(n^2)$ equations for the relevant components. Each force component $F_{i\alpha}$ is a sum of $v_i$ force components with $v_i$ the valency of the vertex $V_i$ i.e. the # of vertices connected to it. Hence each step in (26) involves $n^2v/2$ calculations with

$$v = \sum_{i=1} v_i/n \tag{22}$$

the average valency in the graph.

Let us assume that we need to repeat the process of iterating the dynamics namely (26) or (27) for $s$ steps in order to achieve the goal(s) of the algorithm(s). These goals vary for the various problems of interest. For cluster identification we need the points representing clusters in the graph to physically converge into definable separate regions.

For graph characterizations and comparison we need a fewer number of steps, sufficient to make the distances $r_{ij}(t)$ vary considerably away from their original common value.

The total number of computations involved is $N = O(n^2s)$ if $v$ is finite and $n$ independent or $N = O(n^3s)$ for the extreme case when $v \approx n$. For $N$ not to be polynomial in $n$ we need that $s$ will grow faster than any power of $n$.

In principal one can envision many types of chaotic dynamical evolution where such large number of steps is indeed required.

This is not the case for the first order equations considered here:

$$\dot{\vec{r}}_i = \frac{\vec{F}_i}{\mu} = -\frac{\vec{\nabla}r_i(U)}{\mu}, \tag{23}$$

where the system consistently moves, along the steepest descent, to a minimum of $U$, the potential energy.

If we have a complicated “energy landscape” the system can be trapped in any one of the many local minima, a feature which accounts for the difficulty of protein folding.
neural nets and spin glass problems. The need to keep the same deterministic evolution for $S$ and $S'$ representing $G$ and $G'$ in the first “distortion” algorithm, excludes in our case-the possibility of introducing some stochastic noise to extricate the system from a local minimum.

Fortunately our problem does not allow for many minima. Thus let us fix the locations of all $\vec{r}_i \ i = 1, \ldots, n - 1$ except $\vec{r}_n \equiv \vec{r}$. The velocity $\dot{\vec{r}}(t)$, is dictated by

$$U(\vec{r}) = \sum_{i=1}^{n} C_n U_A(|\vec{r} - \vec{r}_i|) + (1 - C_n) U_R(|\vec{r} - \vec{r}_i|) \quad (24)$$

Assume we have some local equilibrium at $\vec{r}_0$. Locally, in the neighborhood of $\vec{r}_0$, we can use the variables $\rho_i \equiv |\vec{r} - \vec{r}_i| \ i = 1, \ldots, n - 1$, instead of $x_1 \cdots x_{n-1}$ the $n - 1$ Cartesian coordinates of $\vec{r}$. The conditions for an extremum $\vec{\nabla} U(\vec{r}) \ |_{\vec{r}=\vec{r}_0}$ then require that

$$\frac{\partial}{\partial \rho_j} U_A(\rho_j) \ |_{\rho_j=\rho_j^{(o)}} = 0; \quad \text{or} \quad \frac{\partial}{\partial \rho_j} U_R(\rho_j) \ |_{\rho_j=\rho_j^{(o)}} = 0 \quad (25)$$

Thus for generic monotonic $U_A, U_R$, we have no extrema inside the region.

An absolute minimum obtained at the boundary.

**APPLICATIONS OF THE METHOD**

To demonstrate the power of our approach we considered a graph with 100 vertices each of which is randomly connected to seven others. The corresponding connectivity matrix $C$ is shown in Fig.(1). Random reshuffling transforms the $C$ into the matrix $B$ of Fig.(2). Next we applied our algorithm using a combination of attractive and repulsive forces in $n - 1 = 99$ dimensional space. The vertices of the 100-simplex were allowed to move under the influence of the forces on the 98-dimensional hyper-sphere in 99-dimensions. After a number of steps we analyzed the distances between pairs the vertices of the two simplexes. We found perfect correspondence between the distance matrices. We also readily show the permutation matrix which maps one distance matrix on to the another. Applying the latter to the matrix $B$ reproduces exactly the original connectivity matrix $C$ (Fig.(1)).

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FIG. 1: Connectivity matrix for 100 vertices graph with 7 random connections for each vertex.

He would like to dedicate this work to sir Isac Wolfson who donated the chair in theoretical physics at Tel-Aviv University on the occasion of his 80th birthday.

* gudkov@sc.edu
† nussinov@ccsg.tau.ac.il

[1] An analogous physical system was used by Farhi, Goldstone and Gutmann and Sipser arXiv quant-ph/0001106 (2000). Their idea was to create a cave function of $n$ spins satisfying a set of Boolean logic requirements via adiabatic changing of the Hamiltonian.
FIG. 2: Reshuffled connectivity matrix.

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