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LETTER TO THE EDITOR

Graph identification by simulated annealing

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Abstract. A new theoretical approach to graph processing, based on the transformation of a topological graph into a time-dependent periodic melody, is proposed. By using a self-tuning oscillatory dynamical network, graphs can be uniquely reconstructed from their melodies. This opens a perspective for a content-addressable memory invariant under large topology-preserving distortions.

Current interest in the problems of graph processing by dynamical networks has two principal motivations. It is well known that operations with graphs (or semantic nets) should constitute an important property of artificial intelligence (Hogg and Huberman 1987). Generally such operations involve generation, comparison, transformation and communication of graphs by dynamical networks. A closely related problem is the investigation of various physical processes taking place on graphs, such as activation spreading down over a graph (Huberman and Hogg 1987) or decay and diffusion in hierarchically organised systems (Engel *et al* 1988a, b). Another motivation comes from the field of pattern recognition. Although we now have several powerful models of content-addressable memory (Hopfield 1982, Sejnowski *et al* 1986, Gerzon and Mikhailov 1986) they remain very sensitive to topology-preserving distortions. Translation or rotation of an image, its uniaxial stretching or contraction usually result in a loss of recognition. What we often need here is recognition of topological graphs rather than entire pictures.

In this letter I want to propose a new theoretical approach to the processing of topological graphs which is based on their transformation into periodic time-dependent melodies. By using a self-tuning oscillatory network and the technique of simulated annealing (Kirkpatrick *et al* 1983) a graph can be uniquely reconstructed (identified) from its melody.

Any graph is a network of connections between elements. For simplicity, we consider below only the graphs formed by identical elements with symmetric identical connections. If we enumerate all elements in some sequence, such a graph can be specified by its connection matrix T_{ij} , with $T_{ij} = 1$ when the elements i and j are connected, and $T_{ij} = 0$ when the connection is absent. Since connections are symmetric, $T_{ij} = T_{ji}$. It is convenient to put $T_{ii} = 0$.

The definition of a graph by the connection matrix T_{ij} is highly degenerate since it depends on the particular choice of the enumeration sequence. Therefore, for example, the comparison of graphs defined by their connection matrices is an extremely complex problem. In order to find that certain two matrices describe the same graph one should try all possible enumeration sequence permutations and, thus, to perform about $N^2 N!$ elementary operations.

Hence, it is natural to seek a corresponding dynamical system with the dynamics determined only by the pattern of connections and *not* by the enumeration choice.

As an example of such a system we consider a set of identical massive particles tied by elastic strings and allowed to move only along a straight line (i.e. a one-dimensional molecule). Suppose that every particle corresponds to a certain graph element and any two particles are tied by a string only if the corresponding elements of the graph are connected[†].

In this manner any graph can be put into one-to-one correspondence with a certain one-dimensional molecule, described by the dynamical equations

$$\ddot{x}_i = - \sum_{j=1}^N T_{ij}(x_i - x_j) \quad (1)$$

where x_i is the coordinate of the i th particle. (Masses and elasticities are equal to unity.)

Any one-dimensional molecule possesses a definite spectrum of oscillation frequencies $\{\omega_\alpha\}$, $\alpha = 1, \dots, N$, such that $\lambda_\alpha = -\omega_\alpha^2$ are the eigenvalues of the real symmetrical matrix

$$R_{ij} = -T_{ij} + \sum_{k=1}^N T_{ik}\delta_{ij}. \quad (2)$$

Clearly, this spectrum depends only on the pattern of ties in a molecule and not on the enumeration of its particles. What is more important, this spectrum of oscillation frequencies $\{\omega_\alpha\}$ uniquely determines its one-dimensional molecule and hence the graph by which it was generated. This can be seen from the following arguments.

The same set of eigenvalues $\{\lambda_\alpha\}$ would be found for any matrix \mathbf{R}' obtained from \mathbf{R} by some non-degenerate linear transformation \mathbf{U} :

$$\mathbf{R}' = \mathbf{U}^{-1}\mathbf{R}\mathbf{U}. \quad (3)$$

However, this new matrix \mathbf{R}' can be attributed to some one-dimensional molecule, considered above, only if two conditions are satisfied. First, the non-diagonal elements of \mathbf{R}' should be equal only to either -1 or 0 . Second, as follows from (2), any diagonal element of this matrix, taken with the opposite sign, should be equal to the sum of all other elements in the same line (or column, which is the same since the matrix must be symmetric), i.e.

$$R_{ii} = - \sum_{j \neq i} R_{ij}. \quad (4)$$

Examination shows that these two conditions are very stringent and they can be simultaneously met (probably with few exclusions) only if the transformation \mathbf{U} is equivalent to the change of enumeration of lines and columns in the matrix \mathbf{R} , but then \mathbf{R}' would correspond to the same molecule.

Therefore, any graph with N elements can be uniquely specified by the set of N frequencies $\{\omega_\alpha\}$. This is the most compact way it may be specified. Note that if we describe a graph by its connection matrix T_{ij} we should indicate the values of $N(N-1)/2$ independent matrix elements, which reflects the high degeneracy of such a definition.

When a molecule is excited, its oscillations generally represent a superposition of all normal modes. If we take as a time-dependent signal the quantity which is

[†] It should be stressed that this example is purely hypothetical and serves only to demonstrate the principle of graph communication.

proportional to the displacement x_i of a certain particle, it would give us a periodic 'melody' that includes all oscillation frequencies ω_α and hence uniquely specifies the corresponding graph.

Coding into melodies provides a natural way for comparison and recognition of graphs, and for the content-addressable memory invariant under topology-preserving transformations (Mikhailov 1988a).

The next step consists of finding a dynamical system able to solve the inverse problem, i.e. to reconstruct a graph from its melody.

With this purpose let us again consider a one-dimensional molecule but assume that its matrix of connections τ_{ij} is not fixed but mutates randomly in time. Moreover, we assume that oscillations of this molecule are slightly damped and there is an external periodic force $f(t)$ applied to one of the particles.

At fixed connections τ_{ij} this dynamical network is described by the equations

$$\ddot{x}_i = - \sum_{j=1}^N \tau_{ij} (x_i - x_j) - \gamma \dot{x}_i + f(t) \delta_{1i}. \quad (5)$$

Suppose that the periodic force $f(t)$ represents a melody produced by some graph with N elements and is thus characterised by a certain oscillation spectrum $\{\omega_\alpha\}$, and consider a quantity

$$\mathcal{F} = \sum_{i=1}^N \overline{x_i^2(t)} \quad (6)$$

which is obtained by averaging over time intervals including many periods of individual oscillations.

Then, for a given melody $f(t)$ and for a high enough resonance quality ($\omega_\alpha \gg \gamma$), \mathcal{F} is as large as the fit is close between the set of the eigenfrequencies $\{\omega'_\alpha\}$ of the detecting molecule with connections τ_{ij} and the spectrum $\{\omega_\alpha\}$ of the applied melody.

Suppose further that connections τ_{ij} can change randomly in time but these mutations are rather rare: an average interval between two successive mutations is much larger than the relaxation time $t_{\text{rel}} = 1/\gamma$ of the molecule detector. For simplicity we can assume that the mutation probability per unit time is the same for any connection and that the individual mutations (break or creation of a single connection) are independent. We choose the probability of a mutation per unit time as

$$w = A \exp(-\mathcal{F}/\theta) \quad (7)$$

where $A \ll \gamma$.

Such a dynamical network would tend to spend most time in a state with the maximal value of \mathcal{F} which corresponds to the complete coincidence of the sets $\{\omega_\alpha\}$ and $\{\omega'_\alpha\}$. Since every graph uniquely determines a certain set of oscillation frequencies, this implies that the most probable connection pattern in the molecule detector would be identical to the graph generating the applied melody.

The coefficient θ in (7) plays the role of temperature. Due to thermal fluctuations the process of self-tuning cannot stop on a graph that corresponds to some partial resonance. By slowly decreasing the temperature θ we can simulate annealing and ensure that in the final state (at $\theta = 0$) our system would be found with the pattern of connections identical to the original graph.

The aim of the present letter is to outline a general idea of graph coding and identification. Possible practical implementations will be discussed in a separate

publication (Mikhailov 1988b). Note that the proposed model might be easily realised in terms of electrical oscillatory networks with controlled switches.

For computer simulations it is more convenient to use, instead of (7), the Metropolis mutation algorithm (Metropolis *et al* 1953), i.e. to assume that a tentative mutation is always accepted if it results in an increase of \mathcal{F} , and accepted with a small probability proportional to $\exp(\Delta\mathcal{F}/\theta)$ if the change $\Delta\mathcal{F}$ is negative. This algorithm results in better convergence.

Above it was assumed that the total number N' of elements in the detecting dynamical network is the same as the number of elements N in the original graph. It can be easily shown, however, that the network with N' elements can, as well, identify graphs of smaller sizes ($N < N'$). It seems probable that, when the size of the detecting network is not as large as the size of the identified graph ($N > N'$), the result might be a 'skeleton' identification, i.e. the approximate reconstruction of a graph lacking its minor details. This question deserves further investigation.

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