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Could a combinatorial optimization problem be solved by a differential equation?

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Abstract. For the Traveling Salesman Problem (TSP), a combinatorial optimization problem, a feed-forward artificial neural network model, the Continuous Hopfield Network (CHN) model, is used to solve it. This neural network approach is based on the solution of a differential equation. An appropriate parameter setting of this differential equation can assure that the solution is associated with a tour for the TSP.

¿Puede una ecuación diferencial resolver un problema de optimización combinatoria ?

Resumen. El Problema del Viajante puede plantearse a partir del modelo de red neuronal continuo de Hopfield, que determina una solución de equilibrio para una ecuación diferencial con parámetros desconocidos. En el artículo se detalla el procedimiento de determinación de dichos parámetros con el fin de asegurar que la solución de la ecuación diferencial proporcione soluciones válidas para el Problema del Viajante.

1. Introduction

A combinatorial optimization problem can be stated from a finite set of valued objects for which we look for the best (minimum or maximum value) of them. In spite of its very simple structure, there are many of these problems which cannot be solved exactly when dealing with medium or high size instances; this fact can be explained because these problems are classified as NP-hard problems; see Garey and Johnson [2]. The TSP is the most prominent of the unsolved (in the above sense) combinatorial optimization problems and the most common conversational comparator (*Why, it's as hard as the traveling salesman problem!*).

The TSP is an optimization task that arises in many practical situations. It may be stated as follows: given a group of cities to be visited and the distance between any two of them, find the shortest tour that visits each city only once and returns to the starting point.

An Artificial Neural Network (ANN) is a computational paradigm that differs substantially from those based on the *standard* von Neumann architecture. The ANN is inspired by the structure of biological neural networks and their way of encoding and solving problems.

One kind of architecture in neural network modeling is the feed-back, for which the synapses (neural connections) are bidirectional and activation continues until a fixed point has been reached. An example

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of this type of ANN is the Continuous Hopfield Network (CHN), introduced by Hopfield and Tank [4], which mathematically can be viewed as a differential equation with the property that, with an appropriate parameter setting, it converges to a local minimum of the TSP.

Many researchers have investigated the TSP under a neuronal perspective; see, for example, Aiyer [1], Papageorgiou [6] and M.Peng [7]. However, some disappointing results were obtained; the convergence of the network to valid tours for the TSP could not be guaranteed by all of these improvements.

This paper introduces a parameter setting procedure for the CHN applied to the TSP. This procedure is based on the stability conditions of the CHN Energy Function of the valid tours for the TSP. In this way, a set of analytical conditions of the CHN parameters is obtained so that any equilibrium point of the CHN characterizes a tour for the TSP.

The paper is organized as follows: The CHN to solve the TSP is introduced in section 2**.**. Two types of parameter constraints are introduced: those constraints assuring that any tour for the TSP will be an equilibrium point; and, on the other hand, those constraints assuring the non-convergence of any invalid solution for the TSP. As a consequence, each instance of the TSP has its specific parameters, which depend on the number of cities and on the magnitude of the distances. The associated parameter setting is detailed in section 3**.**.

2. Mapping the TSP onto the CHN

The CHN of size n is a fully connected neural network with n continuous valued units. Following the notation of Aiyer *et al.* [1], let $T_{i,j}$ be the strength of the connection from neuron j to neuron i. In addition, each neuron i has an offset bias of i_i^b. If u_i and v_i represent respectively the current state and the output of the unit $i \quad \forall i \in \{1, \ldots, n\}$, let $\mathbf{u}, \mathbf{v}, \mathbf{i}^b$ be the vectors of neuron states, outputs and biases.

The dynamics of the CHN is described by the differential equation:

$$\frac{d\mathbf{u}}{dt} = -\frac{\mathbf{u}}{\tau} + \mathbf{T}\mathbf{v} + \mathbf{i}^b \tag{1}$$

where $\tau > 0$ and the output function $v_i = g(u_i)$ is a hyperbolic tangent

$$g(u_i) = \frac{1}{2}\left(1 + tanh\left(\frac{u_i}{u_0}\right)\right) \quad u_0 > 0 \tag{2}$$

If, for an input vector $\mathbf{u}^0$, there exists a point $\mathbf{u}^e$ such that $\mathbf{u}(t) = \mathbf{u}^e \ \forall t \geq t_e$, for some $t_e \geq 0$, this point is called an equilibrium point of the system defined by differential equation 1. Such an equilibrium point will also be called the limit point of the CHN. The existence of equilibrium points for the CHN is guaranteed if a Lyapunov or Energy function exists. Hopfield [3] showed that, if matrix $\mathbf{T}$ is symmetrical, then the following Lyapunov function exists:

$$E = -\frac{1}{2}\mathbf{v}^t\mathbf{T}\mathbf{v} - (\mathbf{i}^b)^t\mathbf{v} + \frac{1}{\tau}\sum_{i=1}^{N}\int_0^{v_i} g^{-1}(x)dx \tag{3}$$

Following Gee *et al.* [**?**], the CHN will solve those combinatorial problems which can be expressed as the constrained minimization of

$$E = -\frac{1}{2}\mathbf{v}^t\mathbf{T}\mathbf{v} - (\mathbf{i}^b)^t\mathbf{v} \tag{4}$$

which has its extremes at the corners of the n-dimensional hypercube $[0,1]^n$. The idea is that the network's Lyapunov function, when $\tau \longrightarrow \infty$, is associated with the cost function to be minimized in the combinatorial problem. If the value of τ is large, the continuous system performs much like a discrete binary system, ultimately stabilizing with all outputs near zero or one, i.e. the CHN converges to a vertex of the unit hypercube ; see, for example, Wassermann [9].

In this way the CHN output can be used to represent a solution of the combinatorial problem. This process has been termed *mapping* the problem onto the Network and will be explained for the TSP.

Let N be the number of cities and let $d_{x,y}$ be the distance between the cities x and y, with $x, y \in \{1, \ldots, N\}$. A tour of the TSP can be represented by a $N \times N$ permutation matrix, where each row and each column is associated respectively to a particular city and order in the tour. In the following, this concept is formalized: Let

$$H = \{V \in [0,1]^{N \times N}\} \qquad H_C = \{V \in \{0,1\}^{N \times N}\}$$

be respectively the hypercube of $\mathbb{R}^n$, where $n = N \times N$ and its corner set.

Given $V \in H$, let

$$S_i \equiv \sum_x v_{x,i} \qquad S_x \equiv \sum_i v_{x,i} \qquad S \equiv \sum_x \sum_i v_{x,i} = \sum_x S_x = \sum_i S_i$$

be the sum of rows, columns and rows and columns. The tour set for the TSP is:

$$H_T = \{V \in H_C \;/\; S_x = 1, S_i = 1 \; \forall x, i \in \{1, \ldots, N\}\} \tag{5}$$

Based on this representation, Hopfield and Tank [4] proposed the following network mapping, where each neuron of the Network is identified by each element of the above matrix. In this way, there are n neurons, whose output will be denoted as $v_{x,i}$, where $x \in \{1, \ldots, N\}$ is the city index and $i \in \{1, \ldots, N\}$ is the visit order. The matrix $V \in H$ will represent the system state of the CHN. In this way, the Network evolves until it is trapped in some limit or equilibrium point. Obviously, our aim is that this point would be the minimum length tour.

The energy function of the CHN of any state $V \in H$, proposed by Hopfield, is:

$$\begin{aligned} E(V) \;\; = \;\; & \frac{A}{2} \sum_x \sum_i \sum_{j \neq i} v_{x,i} v_{x,j} + \frac{B}{2} \sum_i \sum_x \sum_{y \neq x} v_{x,i} v_{y,i} + \frac{C}{2} \left(\sum_x \sum_i v_{x,i} - N \right)^2 \\ & + \frac{D}{2} \sum_x \sum_{y \neq x} \sum_i d_{x,y} v_{x,i} (v_{y,i+1} + v_{y,i-1}) \end{aligned} \tag{6}$$

(the $i+1$ and $i-1$ subscripts are given modulo N)

The three first terms of the energy function are null for any valid tour for the TSP, the fourth term penalizes the total length of the tour. Comparing them to equation 4, we have

$$E(V) = -\frac{1}{2} \sum_{x,i} \sum_{y,j} v_{x,i} T_{xi,yj} v_{y,j} - \sum_{x,i} i^b_{x,i} v_{x,i} \tag{7}$$

where the weights and thresholds for the CHN are:

$$T_{xi,yj} = -\left(A\delta_{x,y}(1 - \delta_{i,j}) + B(1 - \delta_{x,y})\delta_{i,j} + C + D(\delta_{i,j-1} + \delta_{i,j+1}) d_{x,y} \right) \tag{8}$$

$$i^b_{x,i} = CN \tag{9}$$

The convergence of the neural Network to some point $V \in [0,1]^n$ is related to the partial derivative of its energy function $E(V)$ with respect to $v_{x,i}$ for all $x, i \in \{1, \ldots, N\}$, which will be denoted as

$$E_{x,i}(V) \equiv \frac{\partial E(V)}{\partial v_{x,i}}$$

Taking into account equation 7, $E_{x,i}(V)$ can be computed as

$$E_{x,i}(V) = A(S_x - v_{x,i}) + B(S_i - v_{x,i}) + C(S - N) + D \sum_{y \neq x} d_{x,y} (v_{y,i-1} + v_{y,i+1}) \tag{10}$$

Introducing the following notation:

$$\underline{E}^0(V) \equiv \min_{(x,i)/v_{x,i}=0} E_{x,i}(V) \qquad \overline{E}^1(V) \equiv \max_{(x,i)/v_{x,i}=1} E_{x,i}(V)$$

we can conclude that any point $V \in H$ will be an equilibrium point for CHN if and only if the three following relations

$$\underline{E}^0(V) \geq 0 \tag{11}$$

$$\overline{E}^1(V) \leq 0 \tag{12}$$

$$E_{x,i}(V) = 0 \qquad \forall (x,i) \in \{1,\ldots,N\}^2 \; / \; v_{x,i} \in (0,1) \tag{13}$$

are verified.

3. Parameter setting of the CHN

Any point $V \in H_T$ will be an equilibrium point if and only if relations 11 and 12 are verified. However, with the parameters A, B, C, D, no tour $V \in H_T$ will ever be an equilibrium point for the CHN and another parameter N' is needed. Equation 9 will be replaced by:

$$i^b_{x,i} = CN' \quad \forall x, i \tag{14}$$

and the partial derivative will be computed as

$$E_{x,i}(V) = A(S_x - v_{x,i}) + B(S_i - v_{x,i}) + C(S - N') + D \sum_{y \neq x} d_{x,y}(v_{y,i-1} + v_{y,i+1}) \tag{15}$$

Let d_U and d_L be respectively some upper and lower bounds for the distances $d_{x,y}$:

$$d_L \leq d_{x,y} \leq d_U \qquad \forall x, y \in \{1,\ldots,N\} \tag{16}$$

The following results will be presented without proof, for further details, see Talaván and Yáñez [5].

Theorem 1 *If the energy function parameters for the CHN are nonnegative and verify:*

$$2Dd_U \leq C(N' - N) \leq A + B + Dd_L \tag{17}$$

Then, any tour $V \in H_T$ will be an equilibrium point for the CHN.

Example 1 *Consider the TSP defined by 6 cities on the vertices of a regular hexagon on $\mathbb{R}^2$ with a side length of 2 and with the Euclidean distance.*

The distance matrix is

$$(d_{x,y}) = \begin{pmatrix} 0 & 2 & 2\sqrt{3} & 4 & 2\sqrt{3} & 2 \\ 2 & 0 & 2 & 2\sqrt{3} & 4 & 2\sqrt{3} \\ 2\sqrt{3} & 2 & 0 & 2 & 2\sqrt{3} & 4 \\ 4 & 2\sqrt{3} & 2 & 0 & 2 & 2\sqrt{3} \\ 2\sqrt{3} & 4 & 2\sqrt{3} & 2 & 0 & 2 \\ 2 & 2\sqrt{3} & 4 & 2\sqrt{3} & 2 & 0 \end{pmatrix}$$

From the distance matrix, the following bounds can be obtained:

$$d_L = 2 \qquad d_U = 4$$

It is easy to check that the parameters

$$N' = 8.1 \qquad A = 1.7 \qquad B = 2.2 \qquad C = 1 \qquad D = 0.25$$

verify equations 17:

$$8.1 = N' > N = 6 \quad \textit{and} \quad 2Dd_U = 2 \leq C(N' - N) = 2.1 \leq A + B + Dd_L = 4.4$$

On the other hand, no invalid tour $V \in H - H_T$ can be an equilibrium point for the CHN.

Theorem 2 *If the energy function parameters for the CHN are nonnegative and verify:*

$$3Dd_u - C < C(N' - N) < \min\{B, A + Dd_L, (N-1)A\} \tag{18}$$

Then, any invalid tour $V \in H_C - H_T$ cannot be an equilibrium point.

Theorem 2 gives sufficient conditions so that the CHN will not be trapped in any invalid solution $V \in H_C - H_T$. There could exist, however, some points $V \notin H_C$ (invalid tours consequently) which are also equilibrium points. See the example below.

In example 1, the following values parameters:

$$N' = 8.1 \qquad A = 1.7 \qquad B = 2.2 \qquad C = 1 \qquad D = 0.25$$

verify inequations 18.

However, the point

$$V^e = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0.9 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \quad \in \quad H - H_C$$

is an interior point of the Hamming cube, cannot be a tour for the TSP, and is also a stable point, because it verifies equations 11, 12 and 13.

In this way, inequations 18 of theorem 2 will be substituted by:

$$3Dd_U \leq C(N' - N) \leq \min\{B, A + Dd_L, (N-1)A\} - C \tag{19}$$

respectively.

In example 1, the parameter values of interior stable point V^e verify inequalities 18 and do not verify inequality 19:

$$3Dd_U - C + C(N - N') = -0.1 \in (-C, 0) = (-1, 0)$$

From the inequalities 19, the lower and upper bounds for $C(N' - N)$ of theorem 1, see equations 17, can be substituted by:

$$3Dd_U \leq C(N' - N) \leq \min\{B; A + Dd_L; (N-1)A\} - C \tag{20}$$

One of these parameter can be fixed, say, for instance, $D = \frac{1}{d_U}$. Moreover, the bounds 17 are implied by bounds 20.

As a consequence of the above results, the following parameter setting assure that any stable vertex $V \in H_C$ will be a valid solution of the TSP and also avoiding that any interior point $V \notin H_C$ could be stable.

$$D = \tfrac{1}{d_U} \quad B = 3Dd_U + C \quad A = (3d_U - d_L)D + C = B - Dd_L \quad N' = N + \tfrac{3Dd_U}{C} \tag{21}$$

In example 1, if $C = 1$, the parameter setting 21 gives the following values:

$$D = \frac{1}{d_U} = 0.25 \quad B = 3Dd_U + C = 4 \quad A = B - Dd_L = 3.5 \quad N' = N + \frac{3Dd_U}{C} = 9$$

This parameter setting represents an improvement with respect to other authors in the sense that, not only better solutions are obtained, but —which is the most important feature— valid tours are always obtained. The theoretical results have been tested with sample instances from $TSPLIB$, see Reinelt [8], with sizes of up to 1000 cities. See also Talaván and Yáñez [5] for further details.

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