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Discrete Optimization

The graph coloring problem: A neuronal network approach [☆]

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- Solution of an optimization problem with linear constraints through the **continuous Hopfield network (CHN)** is based on an **energy or Lyapunov function**
- This approach is extended in to optimization problems with **quadratic constraints**.
- As a particular case, the **graph coloring problem (GCP)** is analyzed.

1. Introduction

- ❑ A new energy function that generalizes the function proposed by Hopfield and Tank, can also be used to solve a 0–1 problem with quadratic constraints; this is the case of the graph coloring problem (GCP)
- ❑ With this mapping and an appropriate parameter-setting procedure, valid coloring is **guaranteed**.

2. The continuous Hopfield network (CHN)

A CHN of size n is a fully connected neural network with n continuous valued units. Let T_{ij} be the strength of the connection from neuron j to neuron i . Each neuron i has an offset bias of i_i^b . Let u_i and v_i be, respectively, the current state and the output of the unit $i \forall i \in \{1, \dots, n\}$.

If \mathbf{u} , \mathbf{v} and \mathbf{i}^b represent vectors of the neuron states, outputs and biases, respectively, the dynamics of the CHN is described by the differential equation:

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

and the output function $v_i = g(u_i)$ is a hyperbolic tangent

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

Hopfield [8] showed that if matrix \mathbf{T} is symmetric, then the following Lyapunov function exists:

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

2. The continuous Hopfield network (CHN)

the following sets are needed:

- The Hamming hypercube

$$H \equiv \{\mathbf{v} \in [0, 1]^n\}.$$

- The Hamming hypercube corners set

$$H_C \equiv \{\mathbf{v} \in H : v_i \in \{0, 1\} \quad \forall i = 1, \dots, n\}.$$

- The feasible solutions set

$$H_F \equiv \{\mathbf{v} \in H_C : \mathbf{R}\mathbf{v} = \mathbf{b}\}.$$

An energy function

$$E(\mathbf{v}) = E^O(\mathbf{v}) + E^R(\mathbf{v}) \quad \forall \mathbf{v} \in H$$

$E^O(\mathbf{v})$ is directly proportional to the objective function.

$E^R(\mathbf{v})$ is a quadratic function

We previously proposed the following generalized energy function [16]:

$$E(\mathbf{v}) = \alpha \left\{ \frac{1}{2} \mathbf{v}^t \mathbf{P} \mathbf{v} + \mathbf{q}^t \mathbf{v} \right\} + \frac{1}{2} (\mathbf{R}\mathbf{v})^t \Phi (\mathbf{R}\mathbf{v}) + \mathbf{v}^t \text{diag}(\gamma) (\mathbf{1} - \mathbf{v}) + \beta^t \mathbf{R}\mathbf{v} \quad \forall \mathbf{v} \in H$$

with the parameters $\alpha \in \mathbb{R}$, $\gamma \in \mathbb{R}^n$, $\beta \in \mathbb{R}^m$ and the $m \times m$ matrix parameter Φ .

3. The graph coloring problem

- ❑ From a computational point of view, the GCP is one of the most difficult optimization problems; it is an *NP*-hard problem and the existence of efficient heuristic approaches for the general case cannot be assured.
- ❑ The GCP looks for the lowest number of different colors that can be assigned to the nodes of a graph whereby two nodes cannot share the same color if they are linked by an edge.

3.1. The 0–1 mathematical programming model

So that the GCP can be mapped onto a CHN, it must be expressed as a linear assignment problem with quadratic constraints.

The decision variable is the binary variable:

$$v_{i,k} = \begin{cases} 1 & \text{if } C(i) = k \\ 0 & \text{otherwise} \end{cases} \quad i, k \in \{1, \dots, N\},$$

- ❑ Después aplica las restricciones cuadráticas

3. The graph coloring problem

The more colors that are used, the worse is the objective function. One way to accomplish this idea is through an auxiliary binary variable that takes the value 1 when a particular color has been used:

$$v_{0,k} = \begin{cases} 1 & \text{if the color } k \text{ has been used} \\ 0 & \text{otherwise} \end{cases} \quad k \in \{1, \dots, N\}.$$

the auxiliary variables $v_{0,k}$ can be penalized with the value p_k in the objective function:

$$\min \left\{ \sum_{k=1}^N p_k v_{0,k} \right\}. \quad (11)$$

These constraints can be summarized in the following family of constraints:

$$\sum_{j=1}^{h+1} p_j \geq \sum_{j=1}^h p_{N-j+1} \quad \forall h \in \{1, 2, \dots, \lceil N/2 \rceil\}.$$

From now on, the values of $p_0 = \frac{N}{2}$ and $r = \frac{2}{N}$ are fixed in such a way that the objective function of the linear assignment problem with quadratic constraints is

$$\min \left\{ \sum_{k=1}^N \left(\frac{N}{2} + \frac{2k}{N} \right) v_{0,k} \right\}. \quad (12)$$

4. Generalized energy function for the GCP

To define the energy function for the GCP, the following considerations need to be taken into account so that the mathematical expression of energy function (6) is simplified.

- Only the main diagonal terms of the quadratic matrix parameter Φ are considered; i.e., $\Phi_{j,k} = 0 \forall j \neq k$. In this way, the product of distinct linear constraints is not penalized and the constraints have equal weight: $\Phi_{k,k} = \phi \forall k$.
- The quadratic constraints h^A and h^B are penalized by the parameters ρ^A and $\frac{1}{2}\rho^B$, respectively.
- All linear constraints are equally weighted, where β is the associated parameter.
- The parameters penalizing the non-extreme values of $v_{0,k}$ and $v_{i,k}$ are γ_0 and γ_1 , respectively.

Consequently, the following generalized energy function for the GCP is proposed:

$$E(\mathbf{v}) = \alpha f(\mathbf{v}) + \rho^A h^A(\mathbf{v}) + \frac{1}{2} \rho^B h^B(\mathbf{v}) + \frac{1}{2} \phi \sum_{i=1}^N e_i(\mathbf{v})^2 + \beta \sum_{i=1}^N e_i(\mathbf{v}) + \gamma_0 \sum_{k=1}^N v_{0,k}(1 - v_{0,k}) \\ + \gamma_1 \sum_{i=1}^N \sum_{k=1}^N v_{i,k}(1 - v_{i,k}),$$

5. Parameter setting

Taking into account the particular GPC structure, a direct parameter-setting method, based on the partition of HC-HF, is used.

This method does not depend on the linearity of the constraints.

A feasible solution could be the following:

$$\rho^A = \alpha \left(\frac{N}{2} + 2 \right) + \gamma_0 + \varepsilon,$$

$$\gamma_1 = \frac{\rho^A}{2} + \varepsilon,$$

$$\phi = 2\gamma_1,$$

$$\rho^B = \phi,$$

$$\beta = - \left(\frac{\rho^A}{2} + \phi \right)$$

which depends on the parameters α , γ_0 and ε .

Remark 1. This parameter-setting depends only on the parameter N , the number of nodes of the graph to be colored.

6. Computational experiments

- ❑ The algorithm proposed obtains one equilibrium point for the CHN and is a variable time-step method with a shorter convergence time. Moreover, it is robust with respect to the initial conditions.
- ❑ The graphs to be colored in these computational experiments were chosen from the public library Graph coloring instances following the standards of DIMACS (<http://mat.gsia.cmu.edu/COLOR/instances.html>).
- ❑ The quality of the coloring functions obtained was evaluated in terms of the performance ratio :

$$q = \frac{\text{number of colors used}}{\text{chromatic number}}.$$

6. Computational experiments

Table 1
Computational results of the *Graph coloring instances*

GCP identification	No. of nodes	No. of arcs	Chromatic number	No. of runs	g			Mean time (s)	Mean iterations
					Minimum	Mean	Mode		
MYCIEL3	11	20	4	100	1.00	1.22	1.25	0.20	269.55
MYCIEL4	23	71	5	100	1.40	1.98	2.00	0.36	338.76
QUEEN5_5	25	160	5	100	1.80	2.30	2.40	4.82	5241.55
QUEEN6_6	36	290	7	100	1.43	1.83	1.86	1.17	399.98
MYCIEL5	47	236	6	50	1.00	1.55	1.67	2.34	443.58
QUEEN7_7	49	476	7	50	1.86	2.53	2.57	2.68	438.14
QUEEN8_8	64	728	9	50	2.11	2.55	2.56	6.42	525.1
MYCIEL6	95	755	7	50	1.00	1.21	1.14	26.52	781.76
GAMES120	120	638	9	50	3.22	3.74	3.78	65.34	1032.32
MILES250	128	387	8	25	2.63	3.39	3.38	90.36	1219.92
MILES500	128	1170	20	25	1.90	2.05	1.95	98.76	1218.68
MILES750	128	2113	31	25	1.55	1.74	1.65	88.44	1005.8
MILES1000	128	3216	42	25	1.38	1.51	1.57	91.64	990.84
MILES1500	128	5198	73	25	1.11	1.15	1.12	86.48	955.4
MYCIEL7	191	2360	8	10	1.25	1.78	1.75	417.30	1731.1
MULSO.I.1	197	3925	49	10	1.35	1.43	1.39	511.00	1900.4
LE450_25A	450	8260	25	10	3.64	3.86	4.00	14068.78	4735.89

7. Summary and conclusions

- ❑ In this paper, the generalized energy function we previously introduced was used to solve the GCP.
- ❑ This has been presented as an optimization problem with quadratic constraints.
- ❑ Moreover, to solve the GCP, a set of analytical conditions for the CHN parameters has been deduced