Energy Function-Based Approaches to Graph Coloring

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Introduction

- Undirected graph $G = \{V, E\}$, with N vertices and M edges
- It is represented as an adjacency matrix A_{ij}, where $A_{ij} = 1$ if $\{v_i, v_j\} \in E$ and 0 otherwise.
- Previous coloring neural nets used k binary neurons per vertex to represent its color
- The authors propose using only one neuron with state $S_i \in \{1, \dots, k\}$ or $S_i \in \{0, 1, \dots, k\}$
- An energy function describes the state of the system and the goal is to minimise it

Color update

We will update the network serially, specifically at time $t+1$ a single neuron i will be selected and its state $S(t+1)$ set to a new value c such that

$$\Delta E_i(c,t) \equiv E(S_i(t+1)=c) - E(S_i(t)) < 0. \qquad (1)$$

Thus, the energy will decrease in every time step. So long as the energy function is bounded from below, the network will always converge to a (local) minimum, that is, the network is *globally stable*.

Coloring problem variants

- Minimum coloring (MC): find a partition $V_1, \ldots, V_k$ of V such that connected vertices have different colors (belong to a different partition V_i) for a minimum number of colors k
- Spanning subgraph k-coloring (SSC): minimise the number of improperly colored edges while coloring al the vertices using at most k colors
- Induced subgraph k-coloring (ISC): find the largest set of vertices that can be properly colored using k colors

Energy functions I

$$E_{\mathrm{MC}}(\vec{S}) = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} A_{ij}\delta(S_i, S_j) + \gamma \sum_{i=1}^{N} S_i$$

$$\delta(a,b) = \begin{cases} 1 & \text{if } a = b \\ 0 & \text{otherwise} \end{cases}$$

Energy functions II

$$E_{\mathrm{ISC}}(\vec{S}) = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} A_{ij}\,\mathrm{sgn}(S_i S_j)\delta(S_i, S_j) - \gamma\sum_{i=1}^{N}\mathrm{sgn}(S_i)$$

$$E_{\mathrm{SSC}}(\vec{S}) = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} A_{ij}\delta(S_i, S_j)$$

$$\mathrm{sgn}(x) = \begin{cases} -1 & \text{if } x < 0 \\ 0 & \text{if } x = 0 \\ 1 & \text{if } x > 0. \end{cases}$$

Properties I

we determine a critical value γ^*_{ISC} such that for $\gamma < \gamma^*_{\text{ISC}}$ every local minimum is feasible.

Lemma 1: When $\gamma < \gamma^*_{\text{ISC}} = 1$ all minima of the ISC energy function (3) are feasible solutions.

Properties II

As in the ISC case, we can compute a critical value γ^*_{MC} such that if $\gamma < \gamma^*_{\mathrm{MC}}$ we are guaranteed that every local minimum is a feasible solution.

Lemma 2: When $\gamma < \gamma^*_{\mathrm{MC}} = 1/\Delta(G)$ all minima of the MC energy function (4) are feasible solutions.

Properties III

Lemma 3: Every local minimum of the MC energy function (4) with $\gamma < \gamma^*_{\mathrm{MC}}$ is a minimal coloring.

Properties IV

- Every *minimal-violations* k*-coloring* is represented in some local minimum of the SSC energy function.
- Every *maximal* k*-coloring* is represented in some local minimum of the ISC energy function with $\gamma < \gamma^*_{\mathrm{ISC}}$

Coloring algorithm I

The algorithm has two nested loops, an inner loop and an outer loop. The inner loop starts from a certain initial state and serially updates states until a minimum is reached. The outer loop repeatedly restarts the inner loop from different, randomly chosen, initial states and outputs the best solution found in any restart. The value of the outer loop is in compensating for the limited optimization ability of the inner loop by using multiple restarts.

Coloring algorithm II

```
inner_loop(S⃗, k, γ)
{   ΔE⃗ ← compute_DeltaE(S⃗, k, γ);            // compute initial ΔE⃗
    (i, c) = F(ΔE⃗);                            // pick a first vertex-color pair
    while(i ≠ 0)                              // while an energy decrease is possible
    {   old_c ← S_i;   S_i ← c;               // assign new color c to node i
        update_DeltaE(i, c, old_c, ΔE⃗, γ);    // update ΔE⃗
        (i, c) = F(ΔE⃗);                        // pick next vertex-color pair
    }
    return(S⃗);
}
```

Coloring algorithm III

```
outer_loop(k)
{   S_best ← φ;                                          // initialize best coloring
    γ_H ← find_gammaH(k);                         // set value of γ_H for annealing loop
    for(r ← 1; r ≤ RESTARTS; r ← r + 1)
    {   S ← random_S(k);               // randomly color the given graph with k colors
        S ← annealing_loop(S, k, γ_L, γ_H);              // energy descent with annealing
        if(E(S) < E(S_best))                              // S is the minimum just found
            S_best ← S;                                           // save the best solution
    }
    return(S_best);
}
```

Coloring algorithm IV

We can make different choices of F to embody different heuristics. Note that all will reduce energy. Let $D = \{(i,c) \mid \Delta E_i(c,t) < 0\}$. Reasonable choices of F include:

- *greedy*: F returns the pair $(i,c) \in D$ with the minimum value of $\Delta E_i(c,t) \in D$;
- *random*: F returns any random pair $(i,c) \in D$ with equal probability;
- *probabilistic-greedy*: F returns a pair $(i,c) \in D$ with probability $(|\Delta E_i(c,t)|)/(\sum_{(i',c')\in D} |\Delta E_{i'}(c',t)|)$.

In all cases, F will return $(0,0)$ if D is empty.

Experimental results I

- Benchmark graphs from DIMACS challenge (1993)

Experimental results II

TABLE I

SSC AND ISC PROGRAMS ON SOME OF THE DIMACS COLORING BENCHMARK GRAPHS. IN SSC, v IS THE NUMBER OF VIOLATIONS AND IN ISC n IS THE NUMBER OF COLORED NODES. THE VALUE OF k IS SET EQUAL TO χ OR TO ITS BEST KNOWN APPROXIMATION (IN PARENTHESES). TIMES ARE IN SECONDS ($t[s]$)

Graph				SSC			ISC		
name	$N=\|V\|$	$M=\|E\|$	k	v	$v/M\%$	t [s]	n	$n/N\%$	t [s]
DSJC1000.1	1000	99258	(21)	441.8	0.45	19.7	909.0	90.9	20.6
DSJC1000.5	1000	499652	(84)	738.4	0.15	203.6	858.0	85.8	248.9
DSJC1000.9	1000	898898	(226)	603.8	0.07	735.0	868.2	86.8	1123.2
DSJC250.1	250	6436	(8)	91.8	1.43	0.3	227.5	91.0	0.6
DSJC250.5	250	31336	(28)	140.4	0.45	1.1	218.9	87.6	3.2
DSJC250.9	250	55794	(72)	101.6	0.18	2.8	221.9	88.8	8.0
DSJC500.1	500	24916	(12)	241.4	0.97	2.0	445.2	89.0	2.8
DSJC500.5	500	125248	(48)	320.6	0.26	12.7	433.3	86.7	24.5
DSJC500.9	500	224874	(126)	260.4	0.12	36.7	429.9	86.0	72.1
DSJR500.1	500	7110	12	21.8	0.31	1.1	492.6	98.5	0.6
DSJR500.5	500	117724	(123)	114.4	0.10	12.8	456.6	91.3	18.3
flat1000_50_0	1000	245000	50	2967.0	1.21	157.6	571.6	57.2	256.6
flat1000_76_0	1000	246708	76	999.0	0.40	180.2	815.2	81.5	280.9
flat300_20_0	300	21375	20	613.2	2.87	1.6	222.5	74.2	6.8
flat300_28_0	300	21695	28	250.4	1.15	1.8	246.7	82.2	5.5
fpsol2.i.1	496	11654	65	19.4	0.17	2.2	477.5	96.3	2.9
fpsol2.i.2	451	8691	30	45.6	0.52	1.4	432.7	95.9	1.8
inithx.i.1	864	18707	54	44.2	0.24	7.7	829.8	96.0	6.3
inithx.i.2	645	13979	31	75.2	0.54	3.5	614.6	95.3	3.1
le450_15a	450	8168	15	128.2	1.57	1.2	419.2	93.2	1.5
le450_15c	450	16680	15	567.8	3.40	1.9	351.1	78.0	4.9
le450_25a	450	8260	25	23.4	0.28	1.3	441.9	98.2	1.2
le450_25c	450	17343	25	188.0	1.08	2.1	409.6	91.0	3.9
le450_5a	450	5714	5	584.0	10.22	1.1	432.4	96.1	2.0
le450_5c	450	9803	5	80.8	0.82	1.9	438.2	97.4	1.4
miles1500	128	10396	73	4.4	0.04	0.3	126.6	98.9	0.7
miles250	128	774	8	1.8	0.23	0.1	127.7	99.8	0.1
miles750	128	4226	31	5.6	0.13	0.1	125.9	98.4	0.3
mulsol.i.1	197	3925	49	3.6	0.09	0.3	194.5	98.7	0.4
myciel5	47	236	6	0.0	0.00	0.1	47.0	100.0	0.1
myciel6	95	755	7	0.4	0.05	0.1	95.0	100.0	0.1
myciel7	191	2360	8	0.8	0.03	0.2	190.8	99.9	0.2
queen13_13	169	6656	13	88.4	1.33	0.2	148.3	87.8	0.6
queen14_14	196	8372	(18)	16.6	0.20	0.3	192.2	98.1	0.5
queen15_15	225	10360	(17)	54.4	0.53	0.4	211.1	93.8	0.7
queen16_16	256	12640	(18)	63.2	0.50	0.5	240.4	93.9	1.0
school1	385	19095	14	119.8	0.63	2.2	384.1	99.8	3.5
zeroin.i.1	211	4100	49	9.6	0.23	0.3	202.8	96.1	0.6

Experimental results III

TABLE II

RESULTS FROM SSC- AND ISC-BASED ALGORITHMS (SSC-B AND ISC-B, RESPECTIVELY) FOR MINIMUM COLORING, AND RESULTS FROM MC. TIMES ARE IN SECONDS ($t[s]$) OR, WHEN LONGER THAN ONE HOUR, IN *HOUR: MINUTE* FORMAT

Graph				SSC-B		ISC-B		MC	
name	$\|V\|$	$\|E\|$	χ	k	t [s]	k	t [s]	k	t [s]
DSJC1000.1	1000	99258	(21)	34.4	74.1	34.4	11.6	26.8	6.9
DSJC1000.5	1000	499652	(84)	142.7	887.7	142.7	125.3	111.5	91.7
DSJC1000.9	1000	898898	(226)	351.7	1:21	353.3	1102.4	284.2	394.4
DSJC250.1	250	6436	(8)	13.0	0.7	12.4	0.5	10.5	0.3
DSJC250.5	250	31336	(28)	45.0	5.3	43.9	3.2	36.5	1.9
DSJC250.9	250	55794	(72)	103.2	13.9	102.0	13.5	86.4	5.5
DSJC500.1	500	24916	(12)	20.4	5.6	20.4	2.1	16.0	1.2
DSJC500.5	500	125248	(48)	79.8	63.7	79.5	18.9	63.6	12.2
DSJC500.9	500	224874	(126)	189.1	222.1	192.0	101.6	156.4	41.8
DSJR500.1	500	7110	12	14.1	2.6	14.2	0.8	13.0	0.6
DSJR500.5	500	117724	(123)	161.8	84.9	162.3	38.0	133.5	17.6
flat1000_50_0	1000	245000	50	139.7	938.5	140.7	130.3	108.4	85.2
flat1000_76_0	1000	246708	76	141.0	906.5	140.1	118.6	109.7	100.9
flat300_20_0	300	21375	20	49.6	9.1	49.2	4.6	38.7	2.9
flat300_28_0	300	21695	28	50.5	9.2	49.4	4.9	40.3	2.7
fpsol2.i.1	496	11654	65	96.2	10.3	108.8	5.7	65.0	2.2
fpsol2.i.2	451	8691	30	90.7	5.9	113.1	5.2	30.0	1.4
inithx.i.1	864	18707	54	107.8	54.1	128.0	12.1	54.0	4.2
inithx.i.2	645	13979	31	97.4	23.8	120.4	10.6	31.0	2.6
le450_15a	450	8168	15	22.8	4.9	23.1	2.5	18.0	1.1
le450_15c	450	16680	15	33.1	11.2	33.6	6.0	25.9	2.1
le450_25a	450	8260	25	29.6	4.8	30.3	2.6	25.9	1.2
le450_25c	450	17343	25	39.4	10.0	39.7	5.6	31.0	2.4
le450_5a	450	5714	5	13.4	2.8	13.1	1.1	9.0	0.7
le450_5c	450	9803	5	17.3	4.2	17.4	1.7	5.8	0.7
miles1500	128	10396	73	75.9	1.0	75.9	1.4	73.0	0.9
miles250	128	774	8	8.8	0.1	8.5	0.1	8.0	0.1
miles750	128	4226	31	34.4	0.2	34.2	0.3	31.8	0.3
mulsol.i.1	197	3925	49	52.2	0.9	52.2	1.1	49.0	0.5
myciel5	47	236	6	6.0	0.1	6.0	0.1	6.0	0.1
myciel6	95	755	7	7.0	0.1	7.0	0.1	7.0	0.1
myciel7	191	2360	8	8.2	0.5	8.8	0.4	8.0	0.2
queen13_13	169	6656	13	19.4	0.5	19.1	0.7	16.9	0.4
queen14_14	196	8372	(18)	20.9	0.8	20.3	0.9	18.1	0.5
queen15_15	225	10360	(17)	22.2	1.0	21.8	1.1	19.4	0.6
queen16_16	256	12640	(18)	23.7	1.3	23.6	1.3	21.0	0.7
school1	385	19095	14	45.1	8.9	47.2	4.8	28.3	2.6
zeroin.i.1	211	4100	49	60.4	0.9	61.5	1.0	49.0	0.5

Experimental results IV

TABLE III

A COMPARISON OF MC WITH OTHER NEURAL (RBA) AND NON-NEURAL APPROACHES TO GRAPH COLORING. TIMES ARE IN SECONDS ($t[s]$) OR, WHEN LONGER THAN ONE HOUR, IN *HOUR: MINUTE* FORMAT

Graph		MC		RBA		Coud		lmXRLF	SWO		DSATUR	
name	χ	k	t [s]	k	t [s]	k	t [s]	k	k	t [s]	k	t [s]
DSJC125.5	(17)	21.3	0.4	26	42.0	-	-	18	18.3	1.6	22.9	0.03
DSJC250.5	(28)	36.5	1.9	43	478.0	-	-	30	31.9	8.3	37.3	0.12
DSJC500.5	(48)	63.6	12.2	72	1:47	-	-	50	56.3	40.9	65.7	0.46
DSJC1000.5	(84)	111.5	91.7	127	26:33	-	-	85	101.5	208.6	116.3	1.86
DSJR500.1	12	13.0	0.6	15	907.0	12	0.12	13	12.0	2.0	12.9	0.04
DSJR500.5	(123)	133.5	17.6	143	4:42	-	-	128	124.1	68.7	129.0	0.44
R125.1	5	5.0	0.1	5	6.0	5	0.02	-	5.0	0.2	5.0	0.00
R125.1c	46	46.2	1.0	51	96.0	46	0.13	-	46.0	5.1	46.4	0.05
R125.5	36	38.8	0.5	44	81.0	36	2.60	-	36.0	2.8	38.2	0.03
R250.1	8	8.0	0.2	9	103.0	8	0.05	-	8.0	0.5	8.0	0.01
R250.1c	64	65.8	5.2	76	1133.0	64	2.13	-	64.0	30.6	66.4	0.22
R250.5	65	70.4	2.5	79	1046.0	-	-	-	65.0	14.7	69.1	0.11
R1000.1	20	22.3	2.6	26	3:18	20	0.54	-	20.0	8.0	20.3	0.12
R1000.5	(238)	260.4	156.4	275	56:54	-	-	-	238.9	574.5	249.1	1.79
flat300_20_0	20	38.7	2.9	20	491.0	-	-	20	25.3	16.4	42.1	0.16
flat300_26_0	26	40.4	2.9	26	640.0	-	-	28	35.8	12.0	42.1	0.16
flat300_28_0	28	40.3	2.7	28	690.0	-	-	32	35.7	11.9	41.8	0.16
flat1000_50_0	50	108.4	85.2	50	8:31	-	-	50	100.0	203.9	115.2	1.82
flat1000_60_0	60	109.2	93.9	60	10:8	-	-	61	100.7	198.0	115.1	1.83
flat1000_76_0	76	109.7	100.9	76	13:17	-	-	85	100.6	208.4	114.5	1.83
le450_15a	15	18.0	1.1	22	1162.0	-	-	17	15.0	5.5	17.1	0.07
le450_15b	15	18.0	1.1	22	1168.0	-	-	17	15.0	6.1	16.9	0.07
le450_15c	15	25.9	2.1	30	1694.0	-	-	21	21.1	8.0	24.7	0.14
le450_15d	15	25.9	2.1	31	1766.0	-	-	21	21.2	7.8	24.6	0.14
musol.i.1	49	49.0	0.5	49	379.0	49	0.10	49	49.0	5.9	49.0	0.03
myciel5	6	6.0	0.1	-	-	6	4.17	-	-	-	6.0	0.00
myciel6	7	7.0	0.1	-	-	7	35:22	-	-	-	7.0	0.01
myciel7	8	8.0	0.2	-	-	-	-	8	-	-	8.0	0.02
queen8_8	9	10.6	0.1	-	-	9	38.69	-	-	-	11.6	0.01
queen9_9	10	11.9	0.1	-	-	10	5:12	-	-	-	12.8	0.02
queen15_15	(17)	19.4	0.6	-	-	-	-	17	-	-	20.7	0.08
queen16_16	(18)	21.0	0.7	-	-	-	-	18	-	-	22.1	0.09
school1	14	28.3	2.6	42	2178.0	14	0.41	14	14.0	8.4	18.1	0.15