Grafy a počty - NDMI078	May 2009

Lecture 8

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1 Introduction

We focus on the already mentioned conjecture of Lovász and Plummer regarding the growth of the number of perfect matchings in bridgeless cubic graphs.

Conjecture 1 (Lovász and Plummer, mid-1970s). The number of perfect matchings in a bridgeless cubic graph on n vertices is $2^{\Omega(n)}$.

We briefly mentioned the results known in Lecture 4, and we now consider the conjecture restricted to planar graphs. Chudnovsky and Seymour managed to obtain the following theorem.

Theorem 1 (Chudnovsky and Seymour, 2008)**.** *Every bridgeless cubic planar graph on n vertices contains at least* $2^{n/655978752}$ *perfect matchings.*

To prove Theorem 1, Chudnovsky and Seymour first consider the case where the graph is cyclically 4-connected. Next, they obtain the result for all (bridgeless cubic) planar graphs. In the next lecture, we will see the proof of Theorem 1 for cyclically 4-connected graphs (with a better constant in this case). In this lecture, we explore the links of Conjecture 1 with fullerenes.

2 Fullerenes

A *fullerene* is a cubic carbon molecule in which the atoms are arranged on a sphere in pentagons and hexagons. Since the discovery of the first fullerene molecule [4] in 1985, the fullerenes have been objects of interest to scientists all over the world.

Many properties of fullerene molecules can be studied using mathematical tools and results. Thus, *fullerene graphs* were defined as cubic planar 3-connected graphs with pentagonal and hexagonal faces. Such graphs are suitable models for fullerene molecules: carbon atoms are represented by vertices of the graph, whereas the edges represent bonds between adjacent atoms.

Since all carbon atoms are 4-valent, for every atom precisely one of the three bonds should be doubled. Such a set of double bonds is a *Kekulé structure* in a fullerene. So, the set of doubled bonds in a fullerene is precisely a perfect matching in the corresponding fullerene graph. Let M be a perfect matching in a fullerene graph G. A hexagonal face is *resonant* if it is incident with three edges in M. The maximum size of a set of resonant hexagons in G is the *Clar number* of G.

It turns out that the Clar number is highly related to the stability of the molecule. It is natural to ask whether highly unstable fullerenes can theoretically exist. This question amounts to know whether all fullerene graphs have an exponential number of perfect matchings (in terms of the number of vertices).

The computation of the average number of perfect matchings in fullerene graphs with small number of vertices [12] indicates that this number should grow exponentially with the number p of vertices.

Yet, until 2008, the known general lower bounds for the number of perfect matchings in fullerene graphs were linear in the number of vertices [10, 11, 15]. The best of them asserts that a fullerene graph with p vertices has at least $\left\lceil \frac{3(p+2)}{4} \right\rceil$ different perfect matchings [15]. Moreover, several special classes of fullerene graphs with exponentially many perfect matchings are known. Such classes of fullerene graphs either have the special structure of nanotubes [5], have high symmetry [12] or are obtained using specific operations [13]. Recently, it was finally proved that all fullerene molecules have a linear number of resonant hexagons, hence an exponential number of Kekulé structures [8]. In the next section, we establish this fact.

3 Fullerene graphs have exponentially many perfect matchings

First, we give some definitions. Let $G = (V, E)$ be a cubic graph. A *k-edge-cut* of G is set of k edges the removal of which disconnects G. An edge-cut X is *cyclic* if at least two connected components of $G - X$ contain a cycle. A cyclic edge-cut is *trivial* if at most one connected components of $G - X$ is neither a tree nor a cycle.

It directly follows from the definition that fullerene graphs have no cyclic 4-edge-cuts. On other hand, every fullerene has a trivial cyclic 5-edge-cut, since every fullerene has a face of size 5. Moreover, it was proved that fullerene graphs with non-trivial 5-edge-cuts have a very special structure [5, 9]. To be more precise, they are composed of a pentagon surrounded by a "layer" of five pentagons, then a non-negative number of "layers" of hexagons, and next a "layer" of five pentagons, the outer face being the twelveth pentagon (see Figure 1(a)). If k is the number of layers of hexagons (also called hexagonal rings), then the total number of vertices is $10 \cdot (k + 2)$. Observe that every set composed of precisely one edge between two consecutive layers can be extended to a perfect matching in a natural way. For instance, in Figure 1(b) we see a fullerene graph with two layers of hexagons, and the dashed edges for a set of pre-selected edges containing exactly one edge between any two consecutive layers. The bold edges then show how to extend this matching to a perfect matching. As a result, every fullerene on p vertices with a non-trivial cyclic 5-edge-cut has at least $5^{\frac{p-20}{10}}$ perfect matchings. The interested reader can consult the paper of Qian and Zhang [6] for an exact computation of the number of perfect matchings in those fullerene graphs.

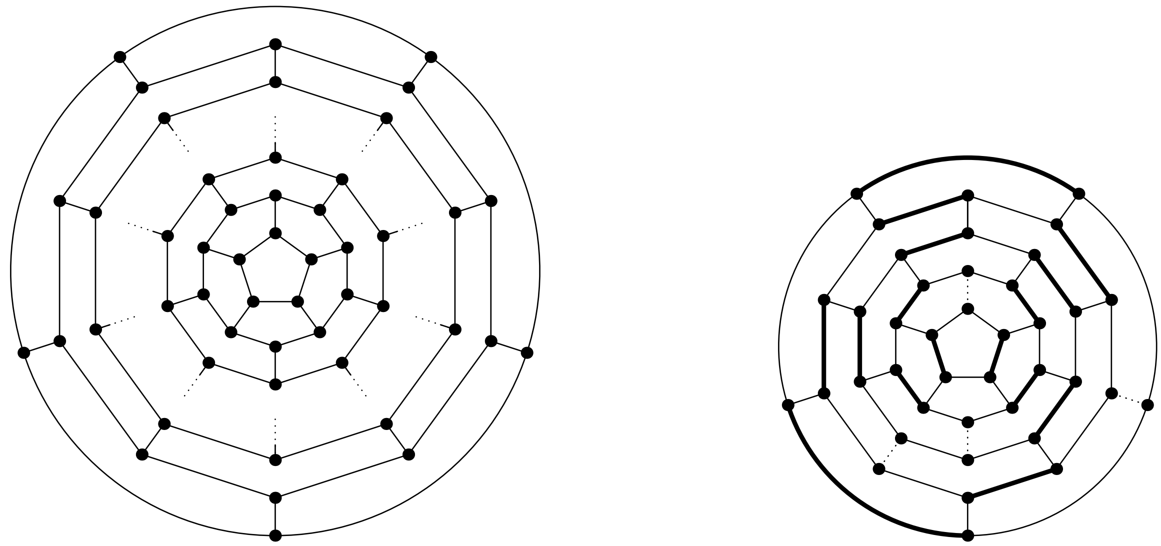

Figure 1: (a) The general shape of fullerene graphs with non-trivial cyclic 5-edge-cuts, and (b) a fullerene with two layers of hexagons, the dashed edges are pre-selected and the bold edges show a completion to a perfect matching.

Note also that such fullerene graphs are Hamiltonian. It is a long-standing open problem to determine whether all fullerene graphs are Hamiltonian.

In the rest, we focus on fullerene graphs with no non-trivial cyclic 5-edge-cuts.

Theorem 2 (Kardoš, Král', Miškuf and Sereni, 2008)**.** *Let G be a fullerene graph with p vertices that has no non-trivial cyclic 5-edge-cut. The number of perfect matchings of G is at least $2^{\frac{p-380}{61}}$.*

Proof. We find a perfect matching M in G such that there are at least $\frac{p-380}{61}$ disjoint resonant hexagonal faces. Since in each such resonant hexagon we can switch the matching to the other edges of the hexagon independently of the other resonant hexagons, the bound will follow immediately.

The dual graph G^* of the graph G is a plane triangulation with 12 vertices of degree 5 and all other vertices of degree 6. Let $U = \{u_1, \ldots, u_{12}\}$ be the set of vertices of degree 5. Our aim is to construct a set W of vertices of G^* of degree 6 and such that:

- the distance between v and v' in G^* is at least 5 for all $v, v' \in W$, $v \neq v'$;
- the distance between v and u in G^* is at least 3 for all $v \in W$ and $u \in U$.

We present a greedy algorithm to construct such a set W. Initially, we set $W_0 = \emptyset$, and we color all the vertices at distance at most 2 from any u_i by the white color. The remaining vertices are colored black. White vertices cannot be chosen as vertices of W. For each $u_i \in U$ there are at most 5 vertices at distance 1 and at most 10 vertices at distance 2. Hence, there are at most $12 \cdot (1+5+10) = 192$ white vertices initially.

Until there are some black vertices, we choose a black vertex v_k and add it to the constructed set, i.e. $W_k := W_{k-1} \cup \{v_k\}$. We recolor all vertices at distance at most 4 from v_k (including v_k) white. Since for any vertex v of degree 6 there are at most $6d$ vertices at distance d, there are at most $1+6+12+18+24 = 61$ new white vertices. This procedure terminates when there are no black vertices.

Let W be the resulting set W_k. The set W contains at least $\frac{f-192}{61}$ vertices where f is the number of faces of G. By Euler's formula, $f = \frac{p}{2} + 2$ and thus $|W| \geq \frac{p-380}{122}$.

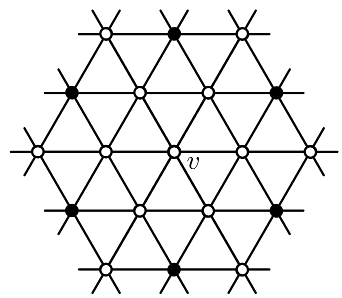

Figure 2: The configuration $R(v)$ and the six vertices in $R^*(v)$.

We next describe how to construct a matching in G with a lot of disjoint resonant hexagons. Given a vertex $v \in W$, let $R(v)$ be the set of vertices at distance at most 2 from v (see Figure 2). The vertices at distance 2 from v form a cycle of length 12 in G^*. This cycle is an induced cycle of G^* since G^* has no non-trivial cyclic 5-edge-cut. Let $R^*(v)$ be the set formed by the 6 independent vertices of $R(v)$ drawn with full circles in Figure 2. Since G has no non-trivial cyclic 5-edge-cut, all the vertices in $R^*(v)$ are different and form an independent set in G^*.

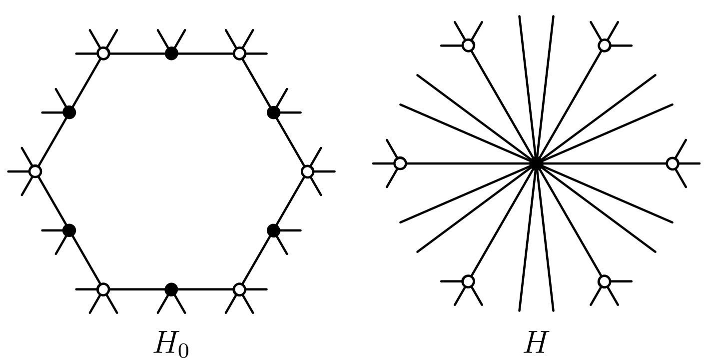

Figure 3: The structure of the graphs H_0 and H.

The sets $R^*(v)$ for $v \in W$ are pairwise disjoint since W only contains vertices at distance at least 5. We now modify the graph G^* to planar graphs H_0 and H. For every vertex $v \in W$, delete v and the six neighbors of v. Let H_0 be the resulting graph. Further identify the six vertices of $R^*(v)$ (see Figure 3). The final plane graph is denoted by H.

The Four Color Theorem[1, 2, 7] asserts the existence of a proper vertex coloring of H using four colors. The coloring of H yields a precoloring of H_0 such that the six vertices of each set $R^*(v)$ have the same color. Let $c(v)$ be this color.

We extend the precoloring of H_0 to a proper coloring of G^*. We first color each vertex v by the color $c(v)$. For each $v \in W$, there are only six uncolored vertices inducing a 6-cycle (the vertices adjacent to v), and each such vertex has three neighbours colored with $c(v)$ and one vertex colored with a different color. Therefore, for each such uncolored vertex, there are 2 available colors. Since every cycle of length six is 2-choosable [3, 14], there is an extension of the coloring of H_0 to G^*. The 4-coloring of G^* corresponds to a proper 3-edge coloring of G. To see this, assume that the vertices of the graph G^* are colored with colors $1, 2, 3$, and 4. There are edges of 6 different color types: 12, 13, 14, 23, 24, and 34. Color the edges of G corresponding to the edges of G^* of types 12 and 34 (which are pairwise disjoint) by the color a, the edges of G corresponding to the edges of G^* of types 13 and 24 by the color b, and the remaining edges, i.e. the edges corresponding to the edges of G^* of types 14 and 23, by the color c. Since the graph G is cubic, each of the color classes a, b, and c forms a perfect matching of G.

Let f be a face corresponding to a vertex w adjacent to $v \in W$ in G^*. Since w has three (non-adjacent) neighbors in G^* colored with the color $c(v)$, the corresponding three non-adjacent edges incident with f are colored with the same color. Hence, the face f is resonant in one of the three matchings formed by the edges of the color a, the edges of the color b, and the edges of the color c.

There are 6 such resonant hexagons for the three matchings for each $v \in W$. Altogether, there are $6|W|$ resonant hexagons. Therefore, one of the matchings has at least $2|W| \geq \frac{p-380}{61}$ resonant hexagons. Observe that the resonant hexagons in one color class are always disjoint: if they were not disjoint, they would correspond to two adjacent neighbors w and w' of some vertex $v \in W$. But the colors assigned to w and w' are different, in particular, the edges corresponding to vw and vw' have different colors. Hence, the hexagons corresponding to w and w' are resonant for different colors a, b, or c. The desired bound on the number of perfect matchings readily follows. $\square$

Theorem 2 combined with the lower bound of $5^{\frac{p-20}{10}}$ derived earlier on the number of perfect matchings in fullerene graphs with non-trivial cyclic 5-edge cuts yields the following.

Corollary 3. *Every fullerene graph with p vertices has at least $2^{\frac{p-380}{61}}$ perfect matchings.*

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