ENTROPY BOUNDS FOR PERFECT MATCHINGS AND HAMILTONIAN CYCLES*

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For a graph G = (V, E) and $\mathbf{x} : E \to \mathbb{R}^+$ satisfying $\sum_{e \ni v} \mathbf{x}_e = 1$ for each $v \in V$, set $h(\mathbf{x}) = \sum_e \mathbf{x}_e \log(1/\mathbf{x}_e)$ (with $\log = \log_2$). We show that for any n-vertex G, random (not necessarily uniform) perfect matching \mathbf{f} satisfying a mild technical condition, and $\mathbf{x}_e = \Pr(e \in \mathbf{f})$,

$$H(\mathbf{f}) < h(\mathbf{x}) - \frac{n}{2}\log e + o(n)$$

(where H is binary entropy). This implies a similar bound for random Hamiltonian cycles. Specializing these bounds completes a proof, begun in [6], of a quite precise determination of the numbers of perfect matchings and Hamiltonian cycles in Dirac graphs (graphs with minimum degree at least n/2) in terms of $h(G) := \max \sum_e \mathbf{x}_e \log(1/\mathbf{x}_e)$ (the maximum over \mathbf{x} as above). For instance, for the number, $\Psi(G)$, of Hamiltonian cycles in such a G, we have

$$\Psi(G) = \exp_2[2h(G) - n\log e - o(n)].$$

1. Introduction

Our main result is Theorem 1.2. We begin by recalling a statement from [6], completion of whose proof was the original motivation for the present work. For a graph G = (V, E) and edge weighting $\mathbf{x} : E \to \Re^+$, set $h(\mathbf{x}) = \sum_e \mathbf{x}_e \log(1/\mathbf{x}_e)$ (where $\log = \log_2$). We will call this the *entropy* of \mathbf{x} (but note it is not really entropy since $\sum \mathbf{x}_e$ will not usually be 1). Call an edge weighting \mathbf{x} proper if $\sum_{e\ni v} \mathbf{x}_e = 1$ for each $v \in V$. (Such an \mathbf{x} is often called a "perfect fractional matching".) Finally, let h(G) (the "entropy" of G) be the

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maximum of $h(\mathbf{x})$ over proper edge weightings \mathbf{x} . (In the absence of proper weightings we may set h(G) = 0, but this won't be an issue here.)

We use $\Phi(G)$ and $\Psi(G)$ for the numbers of perfect matchings and Hamiltonian cycles of a graph G. Recall that a graph is Dirac if it has minimum degree at least n/2. (The reference is of course to [7], which proves that such graphs are Hamiltonian.)

Theorem 1.1. For any n-vertex Dirac graph G,

(1)
$$\log \Psi(G) = 2h(G) - n\log e - o(n),$$

(note o(n) is not necessarily positive), and, if n is even,

(2)
$$\log \Phi(G) = h(G) - (n/2) \log e - o(n).$$

The lower bounds (that is, that the l.h.s.'s of (1) and (2) are larger than the r.h.s.'s) were proved in [6]. Of course the second follows from the first, since, trivially, $2\Psi(G) \leq \Phi^2(G)$ for any G with an even number of vertices. One perhaps surprising consequence of Theorem 1.1 is that for Dirac graphs this inequality is close to the truth, namely

$$\Psi(G) = e^{-o(n)}\Phi^2(G).$$

(Throughout our discussion n is the default for |V(G)|.)

When combined with a lower bound on h(G) proved in [6], the lower bound in (1) says in particular that for any (n-vertex) Dirac G,

(3)
$$\Psi(G) \ge n!/(2 + o(1))^n;$$

this proved a conjecture from [12] which was the starting point for [6] and the present work.

The upper bounds in Theorem 1.1 are essentially instances of the next result. We regard a perfect matching as either an involution $f: V \to V$ (in the obvious way), or as a set of edges.

Theorem 1.2. For any n-vertex graph G:

(a) if **f** is a random (not necessarily uniform) perfect matching of G and $\mathbf{x}_e = \Pr(e \in \mathbf{f})$ for $e \in E$, then

(4)
$$H(\mathbf{f}) < h(\mathbf{x}) - \frac{n}{2}\log e + o(n)$$

provided

(5)
$$\sum \mathbf{x}_e^2 \log(2/\mathbf{x}_e) < o(n);$$

(b) if **C** is a random Hamiltonian cycle of G and $\mathbf{x}_e = \frac{1}{2} \Pr(e \in \mathbf{C})$ satisfies (5), then

(6)
$$H(\mathbf{C}) < 2h(\mathbf{x}) - n\log e + o(n).$$

Recall that Brégman's Theorem [2] says (in graph-theoretic language) that for a bipartite graph G on vertex set $X \cup Y$, one has

(7)
$$\log \Phi(G) \le \sum_{x \in X} \frac{1}{d_x} \log d_x!$$

(where d_x is the degree of x). This is sharp for any disjoint union of complete, balanced bipartite graphs. A nonbipartite version, which is sharp for the same examples, says¹: for any G,

(8)
$$\log \Phi(G) \le \sum_{v \in V(G)} \frac{1}{2d_v} \log d_v!.$$

The l.h.s. of (7) is trivially at most $\sum \log d_x$, while that of (8) is at most $\frac{1}{2}\sum \log d_v$ – an application of *Shearer's Entropy Lemma* ([3, p. 33], but see e.g. [9, Lemma 2.1] for the relevant form) to $\log \Phi(G) = H(\mathbf{f})$, with \mathbf{f} a uniform (random) perfect matching (and H binary entropy; for entropy basics see [10] or [4]). Thus for large degrees, each of (7), (8) gains about $\log e$ per vertex.

Theorem 1.2 does something similar in a more general setting, but with a small loss of precision. Though the error makes no difference for Theorem 1.1, it would be nice to have versions of Theorem 1.2 that include (7) and (8). Let $\varphi(x) = 2^{-x} \log \Gamma(2^x + 1)$ (so $\varphi(\log d) = d^{-1} \log d!$ for positive integer d). Could it be that for a general (i.e., not necessarily uniform) random perfect matching \mathbf{f} , (7) and (8) extend to

$$H(\mathbf{f}) \le \sum_{x \in X} \varphi(H(\mathbf{f}(x)))$$

and

$$H(\mathbf{f}) \le \frac{1}{2} \sum_{v} \varphi(H(\mathbf{f}(v)))$$
?

¹ This was proved, but not published, a few years ago by L. Lovász and the second author, and has since appeared in [8] and [1].

2. Proof of Theorem 1.1

To see that Theorem 1.2 implies the upper bounds in Theorem 1.1, we need to show that (5) holds when G is Dirac and \mathbf{f} (resp. \mathbf{C}) is a uniform perfect matching (resp. Hamiltonian cycle). (Note it is not necessarily true here that all \mathbf{x}_e 's are small. Suppose for instance that V(G) is the disjoint union of A and B, each of size n/2, and E(G) consists of a single edge e contained in A together with all edges not contained in A. Then for \mathbf{f} a uniform perfect matching and \mathbf{x} as above we have $\mathbf{x}_e = 1/3$.)

The verifications of (5) in these two cases (uniform \mathbf{f} , uniform \mathbf{C}) are essentially identical, so we just consider the first. Note that (5) is equivalent to the statement that for some $\alpha = o(1)$ we have $\sum \{\mathbf{x}_e : \mathbf{x}_e \geq \alpha\} < o(n)$. (This obviously implies (5). For the converse, let $f(\alpha) = \sum \{\mathbf{x}_e : \mathbf{x}_e \geq \alpha\}$ and $\alpha_0 = \max\{\alpha : f(\alpha) \geq \alpha n\}$. Then (i) for $\alpha = \alpha_0$, $o(n) > \sum \mathbf{x}_e^2 \geq (f(\alpha)/\alpha)\alpha^2 = \alpha f(\alpha) \geq \alpha^2 n$ implies $\alpha_0 < o(1)$, and (ii) for any α with $\alpha_0 < \alpha < o(1)$, we have $f(\alpha) < \alpha n < o(n)$.)

Assume then that $\alpha = \alpha(n)$ is both $\omega(1/\sqrt{\log n})$ and o(1), and suppose for a contradiction that \mathcal{B} is a set of αn edges, each of weight at least α , and let $\sum_{e \in \mathcal{B}} \mathbf{x}_e = \gamma n$; thus $\alpha^2 \leq \gamma \leq \alpha$. Then Shearer's Lemma and concavity of $h(z) := z \log(1/z)$ give

$$H(\mathbf{f}) \leq \frac{1}{2} \sum_{v \in V} H(\mathbf{f}(v)) = h(\mathbf{x})$$

$$= \sum_{e \in \mathcal{B}} h(\mathbf{x}_e) + \sum_{e \notin \mathcal{B}} h(\mathbf{x}_e)$$

$$\leq \alpha n h\left(\frac{\gamma n}{\alpha n}\right) + \left(\binom{n}{2} - \alpha n\right) h\left(\frac{n/2 - \gamma n}{\binom{n}{2} - \alpha n}\right)$$

$$< \alpha n + (1/2 - \gamma)n(\log n - \log(1 - 2\gamma))$$

$$< (1/2 - \gamma)n\log n + 3\alpha n = (n/2)(\log n - \omega(1)).$$

But we know from (3) that $H(\mathbf{f}) > (n/2)(\log(n/2) - \log e - o(1))$, and this gives the desired contradiction.

3. Proof of Theorem 1.2

Observe, first of all, that (a) easily implies (b). To see this for even n, let \mathbf{f} be the random matching gotten by first choosing \mathbf{C} and then choosing each of the two perfect matchings contained in \mathbf{C} to be \mathbf{f} with probability 1/2.

Then the \mathbf{x} in (a) is the same as that in (b). On the other hand, since the laws of \mathbf{f} and $\mathbf{C} \setminus \mathbf{f}$ are the same, we have

$$H(\mathbf{C}) + 1 = H(\mathbf{f}, \mathbf{C} \setminus \mathbf{f}) \le 2H(\mathbf{f}),$$

so that (6) follows from (4).

When n is odd, we have a simple reduction to the even case: Let G' be gotten from G by adding a new vertex z adjacent to all vertices of G, and let \mathbf{C}' be the random Hamiltonian cycle of G' gotten by choosing an edge xy uniformly from \mathbf{C} and replacing it by the path (x, z, y). Then for $\mathbf{x}'_e = \frac{1}{2} \Pr(e \in \mathbf{C}')$ we have

$$\mathbf{x}'_e = \begin{cases} (1 - 1/n)\mathbf{x}_e & \text{if } e \in E(G) \\ 1/n & \text{if } z \in e, \end{cases}$$

whence

$$h(\mathbf{x}') = \sum_{e \in E(G)} \left(1 - \frac{1}{n}\right) \mathbf{x}_e \log \frac{n}{(n-1)\mathbf{x}_e} + n \cdot \frac{1}{n} \log n < h(\mathbf{x}) + \log n + 1.$$

On the other hand (noting \mathbf{x}' clearly satisfies (5)),

$$H(\mathbf{C}) = H(\mathbf{C}') - \log n < 2h(\mathbf{x}') - (n+1)\log e + o(n) - \log n,$$

and combining the last two observations again gives (6).

We now turn to (a). Our approach here is similar to Radhakrishnan's in [11] (which is in turn similar to Schrijver's [13], but the entropy viewpoint of [11] is surely the correct one). A key difference is that we cannot afford to bound the summand in (9) by the log of the number of possibilities for $\mathbf{f}(v)$ given \mathbf{Y}_v , as one would at a corresponding point in [11].

Note that we may assume $G = K_n$ (since we may simply regard \mathbf{f} as a random matching of K_n that makes no use of edges not belonging to G). Strangely, this trivial assumption yields a significant simplification of the original proof of (a) given in [5].

We use f_B for the restriction of f to $B \subseteq V$. For a permutation σ of V and $v \in V$, set $B(\sigma, v) = \{w \in V : \sigma(w) < \sigma(v)\}$. Let \mathbf{s} be a random (uniform) permutation of V and $\mathbf{Y}_v = (\mathbf{s}, \mathbf{f}_{B(\mathbf{s},v)})$. Then (by the "chain rule")

$$H(\mathbf{f}) = \frac{1}{n!} \sum_{\sigma} \sum_{v} H(\mathbf{f}(v) \mid \mathbf{f}_{B(\sigma,v)})$$

$$= \sum_{v} \sum_{\sigma} \sum_{g} \frac{1}{n!} \Pr(\mathbf{f}_{B(\sigma,v)} = g) H(\mathbf{f}(v) \mid \sigma, g)$$

$$= \sum_{v} H(\mathbf{f}(v) \mid \mathbf{Y}_{v}),$$
(9)

where σ ranges over possible values of **s** and, given σ , g ranges over possible values of $\mathbf{f}_{B(\sigma,v)}$ (and the conditioning on (σ,g) has the obvious meaning).

Now let

$$\mathbf{Z}_v = \begin{cases} (\{\mathbf{f}(v)\}, \Lambda) & \text{if } \mathbf{s}(\mathbf{f}(v)) < \mathbf{s}(v) \\ V \setminus \{v\} \setminus (B(\mathbf{s}, v) \cup \mathbf{f}(B(\mathbf{s}, v))) & \text{otherwise.} \end{cases}$$

This is basically the set of possibilities remaining when we come to specify $\mathbf{f}(v)$ (following the ordering \mathbf{s}), but it will be helpful to distinguish the two ways in which this set can be a singleton $\{y\}$ (namely we can have $\mathbf{f}(v) = y$ with $\mathbf{s}(y) < \mathbf{s}(v)$ or with $\mathbf{s}(y) > \mathbf{s}(v)$ and $V \setminus \{v\} \setminus (B(\mathbf{s}, v) \cup \mathbf{f}(B(\mathbf{s}, v))) = \{y\}$).

Since \mathbf{Z}_v is a function of \mathbf{Y}_v , we have $H(\mathbf{f}(v) | \mathbf{Y}_v) \leq H(\mathbf{f}(v) | \mathbf{Z}_v)$ and so (by (9))

(10)
$$H(\mathbf{f}) \le \sum_{v} H(\mathbf{f}(v) \mid \mathbf{Z}_v).$$

Our main task is bounding $H(\mathbf{f}(v)|\mathbf{Z}_v)$.

From this point we fix v and write \mathbf{Z} in place of \mathbf{Z}_v . We use y for values of $\mathbf{f}(v)$ and Z for values of \mathbf{Z} not of the form $(\{\mathbf{f}(v)\}, \Lambda)$. We use p_y for $\Pr(\mathbf{f}(v)=y)$, but apart from this let $\Pr(Z)=\Pr(\mathbf{Z}=Z)$, $\Pr(Z\mid y)=\Pr(\mathbf{Z}=Z\mid \mathbf{f}(v)=y)$ and so on.

Since $H(\mathbf{f}(v) | \mathbf{Z} = (y, \Lambda)) = 0$, we have

$$H(\mathbf{f}(v) \mid \mathbf{Z}) = \sum_{Z} \Pr(Z) \sum_{y} \Pr(y \mid Z) \log \frac{1}{\Pr(y \mid Z)}$$

$$= \sum_{y} \sum_{Z} \Pr(y, Z) \log \frac{\Pr(Z)}{\Pr(y, Z)}$$

$$= \sum_{y} p_{y} \left[\frac{1}{2} \log \frac{1}{p_{y}} + \sum_{Z} \Pr(Z \mid y) \log \frac{\Pr(Z)}{\Pr(Z \mid y)} \right]$$

$$= \frac{1}{2} H(\mathbf{f}(v)) + \sum_{y} p_{y} \sum_{Z} \Pr(Z \mid y) \log \frac{\Pr(Z)}{\Pr(Z \mid y)}.$$
(12)

(For (11) notice that, for any y, $\sum \Pr(Z \mid y) = 1/2$, since $\mathbf{f}(v)$ and the event $\{\mathbf{s}(\mathbf{f}(v)) < \mathbf{s}(v)\}$ are independent.) We want to show that the second term in (12) is at most about $(-\log e)/2$. (Note $\sum H(\mathbf{f}(v)) = 2h(\mathbf{x})$.)

Fix $y \in V \setminus \{v\}$ with $p_y > 0$. Let Q be the event $\{\mathbf{s}(\mathbf{f}(v)) > \mathbf{s}(v)\}$, and for $k \in \{1, ..., n-1\}$, set

$$q_k = \sum \{ \Pr(Z \mid y) \colon Z \ni y, |Z| = k \} = \Pr(Q, |\mathbf{Z}| = k \mid \mathbf{f}(v) = y),$$

 $r_k = \sum \{ \Pr(Z) \colon Z \ni y, |Z| = k \} = \Pr(Q, |\mathbf{Z}| = k, \mathbf{Z} \ni y).$

(Notice that " $|\mathbf{Z}| = k$ " and " $\mathbf{Z} \ni y$ " make sense once we know Q holds, and that it is not really necessary to specify " $Z \ni y$ " in the definition of q_k .) We have

$$\sum_{Z} \Pr(Z \mid y) \log \frac{\Pr(Z)}{\Pr(Z \mid y)} \\
= \sum_{k} q_{k} \sum_{k} \left\{ \frac{\Pr(Z \mid y)}{q_{k}} \log \frac{\Pr(Z)}{\Pr(Z \mid y)} : Z \ni y, |Z| = k \right\} \\
(13) \qquad \leq \sum_{k} q_{k} \log \frac{r_{k}}{q_{k}},$$

so that (noting $p_y = \mathbf{x}_{vy}$) Theorem 1.2 will follow from

(14)
$$\sum_{k} q_k \log \frac{r_k}{q_k} < -\frac{1}{2} \log e + O(p_y \log(2/p_y) + n^{-1} \log n).$$

The values of q_k and r_k are as follows. Let

$$s_k = \Pr(Q, |\mathbf{Z}| = k, \mathbf{Z} \ni y \mid \mathbf{f}(v) \neq y).$$

Then $r_k = p_y q_k + (1 - p_y) s_k$ and (with justifications to follow) we have

(15)
$$q_k = \begin{cases} 1/n & \text{if } k = 1, 3, \dots, n-1 \\ 0 & \text{otherwise} \end{cases}$$

and

(16)
$$s_k = \begin{cases} \frac{k-1}{n(n-2)} & \text{if } k = 1, 3, \dots, n-1 \\ 0 & \text{otherwise.} \end{cases}$$

In fact these identities hold even if we condition on the value of \mathbf{f} ; that is, (15) is still correct if we replace q_k by

$$q_k(f) = \Pr(Q, |\mathbf{Z}| = k \mid \mathbf{f} = f)$$

for any f (but we only use this when f(v) = y), and (16) is correct with s_k replaced by

$$s_k(f) = \Pr(Q, |\mathbf{Z}| = k, \mathbf{Z} \ni y \mid \mathbf{f} = f)$$

provided $f(v) \neq y$. (Given $\{\mathbf{f} = f\}$ and Q we may order the edges of f by letting e precede e' if the first vertex of e (under the random permutation \mathbf{s}) precedes that of e'. Then $|\mathbf{Z}| - 1$ is twice the number of edges of f that follow the edge containing v in this order, and this number is uniform from $\{0, \ldots, n/2-1\}$; and then, given $|\mathbf{Z}|$, each vertex other than v and f(v) – in particular y if $f(v) \neq y$ – is equally likely to belong to \mathbf{Z} .)

Thus,

$$\sum_{k} q_{k} \log \frac{r_{k}}{q_{k}} = \frac{1}{n} \sum_{t=1}^{n/2} \log \left[p_{y} + (1 - p_{y}) \frac{2t - 2}{n - 2} \right]$$

$$\leq \frac{1}{2n} \sum_{l=2}^{n} \log [p_{y} + (1 - p_{y})l/n]$$

$$= \frac{1}{2n} \sum_{l=2}^{n} \log (l/n) + \frac{1}{2n} \sum_{l=2}^{n} \log (1 + p_{y}(n/l - 1))$$

$$< -\frac{1}{2} \log e + O(n^{-1} \log n) + \frac{1}{2n} \sum_{l=2}^{n} \log (1 + p_{y}n/l).$$
(17)

For the last sum we have

$$\sum_{l=2}^{n} \log(1 + p_y n/l) < \sum_{2 \le l \le p_y n} \log(2p_y n/l) + \log e \sum_{l > p_y n} p_y n/l < p_y n \log(2e) + p_y n \log(1/p_y),$$

so that the expression in (17) is less than

$$-\frac{1}{2}\log e + O(p_y \log(2/p_y) + n^{-1}\log n),$$

and we have (14).

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