The Generalised Randić Index of Trees

Paul Balister*§ Béla Bollobás†§ Stefanie Gerke‡§

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Abstract

The Generalised Randić index $R_{-\alpha}(T)$ of a tree T is the sum over the edges uv of T of $(d(u)d(v))^{-\alpha}$ where $d(x)$ is the degree of the vertex x in T. For all $\alpha > 0$, we find the minimal constant $\beta_c = \beta_c(\alpha)$ such that for all trees on at least 3 vertices $R_{-\alpha}(T) \leq \beta_c(n+1)$ where $n = |V(T)|$ is the number of vertices of T. For example, when $\alpha = 1$, $\beta_c = \frac{15}{56}$. This bound is sharp up to the additive constant — for infinitely many n we give examples of trees T on n vertices with $R_{-\alpha}(T) \geq \beta_c(n-1)$. More generally, fix $\gamma > 0$ and define $\tilde{n} = (n - n_1) + \gamma n_1$, where $n = n(T)$ is the number of vertices of T and $n_1 = n_1(T)$ is the number of leaves of T. We determine the best constant $\beta_c = \beta_c(\alpha, \gamma)$ such that for all trees on at least 3 vertices, $R_{-\alpha}(T) \leq \beta_c(\tilde{n}+1)$. Using these results one can determine (up to $o(n)$ terms) the maximal Randić index of a tree with a specified number of vertices and leaves. Our methods also yield bounds when the maximum degree of the tree is restricted.

1 Introduction

In this paper we consider the generalized Randić index of a tree. For a constant α, the generalized Randić index $R_{-\alpha}(T)$ of a tree T is the sum of $(d(u)d(v))^{-\alpha}$ over all edges uv of T where $d(x)$ is the degree of x. The Randić indices R_{-1} and $R_{-1/2}$ were introduced by

*Department of Mathematical Sciences, University of Memphis, TN 38152-3240, USA. E-mail: pbalistr@memphis.edu

†Trinity College Cambridge, CB2 1TQ, UK, and University of Memphis, TN 38152-3240, USA. E-mail: B.Bollobas@dpmms.cam.ac.uk

‡Institute of Theoretical Computer Science, ETH Zurich, 8092 Zurich, Switzerland. E-mail: sgerke@inf.ethz.ch

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Randić in [9] to give a theoretical characterization for molecular branching. Due to the tree-like structures of the molecules of interest, the generalized Randić index has been studied most extensively for trees [2, 3, 4, 5, 6, 7, 8, 10]. It is known that for any tree T on $n \geq 3$ vertices, $R_{-1/2}(T) \leq \frac{n}{2} + \sqrt{2} - \frac{3}{2}$, and that this bound is achieved when T is a path [8]. It was shown in [4] that $R_{-1}(T) \leq \frac{15}{56}n + 11$. Examples previously given in [2] show that this upper bound is best possible except for the constant term. For $\alpha \notin (1/2, 2)$, trees on n vertices with maximal Randić index were exhibited in [3]. Weaker upper bounds for all $\alpha > 0$ were shown in [7] where the bounds were given in terms of $n = |V(T)|$ and the number n_1 of leaves. We extend these results by finding for every $\alpha, \gamma > 0$, an effectively computable constant $\beta_c = \beta_c(\alpha, \gamma)$ such that for all trees T on $n \geq 3$ vertices with n_1 leaves, $R_{-\alpha}(T) \leq \beta_c(\tilde{n}+1)$, where $\tilde{n} = (n-n_1)+\gamma n_1$; see Theorem 5. The constant γ will enable us later to give good upper bounds if we are only interested in trees with a certain proportion of leaves; for details see Section 4. For $0 < \gamma \leq 2^\alpha$, we construct infinitely many trees such that $R_{-\alpha}(T) \geq \beta_c(\tilde{n} - 1)$ showing that the upper bound is best possible up to the constant term. Let us remark that there are examples of trees T with $R_{-\alpha}(T) > \beta_c(\alpha, \gamma)\tilde{n}$ and thus some positive constant term is needed. For $\gamma \geq 2^\alpha$ it follows from our results that $\beta_c = 4^{-\alpha}$, and the family of paths shows that one cannot improve β_c.

Our methods also allow us to take the maximum degree Δ of the tree into account. For every $\alpha, \gamma > 0$, we find an effectively computable constant $\beta_\Delta(\alpha, \gamma)$ such that for all trees T of maximum degree Δ, $R_{-\alpha}(T) \leq \beta_\Delta(\alpha, \gamma)\tilde{n} + C$ for some constant $C = C(\Delta)$; see Theorem 6. These results extend the results in [10] where $\Delta = 3$, $\gamma = \alpha = 1$ was considered, and the results in [5, 6] where they treated the case $\Delta = 4$ (or *chemical* trees), $\gamma = 1$ and $\alpha = 1$ or $\alpha < 0$.

In Section 2 we introduce the necessary notation to define $\beta_c = \beta_c(\alpha, \gamma)$. In Section 3 we prove that $\beta_c(\tilde{n} + 1)$ is in fact an upper bound on the Randić index $R_{-\alpha}(T)$ for all trees with $n \geq 3$ vertices and n_1 leaves. In Section 4 we exhibit infinitely many trees T with $R_{-\alpha}(T) \geq \beta_c(\tilde{n} - 1)$. In Section 5 we discuss how to calculate β_c effectively and give examples of $\beta_c(\alpha, \gamma)$ for some specific values of α and γ.

2 Notation and Preliminaries

Define a *half-tree* to be a tree T with one "dangling" edge added that is attached to a vertex v_0 of T, but to no other vertex; see Figure 1. We call v_0 the *root* of T. We say that T is trivial if it consists of just v_0 and the dangling edge. Given any tree with an edge uv, we can construct two half-trees by cutting the tree at the edge uv. Similarly, any two half-trees can be joined via their dangling edges to form a tree. Fix $\alpha > 0$. We define the Randić index $R_{-\alpha}(T)$ of a half-tree by summing $(d(u)d(v))^{-\alpha}$ over all the non-dangling edges uv of T. Note that the dangling edge does not contribute directly to the sum defining $R_{-\alpha}(T)$, but it does affect $R_{-\alpha}(T)$ since we include it in the degree count $d(v_0)$ of the vertex v_0.

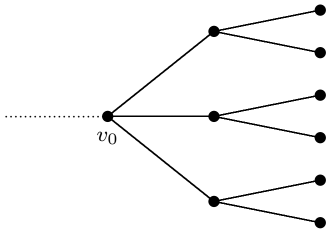

Figure 1: The half-tree $[4, 3, 1]$ with root v_0.

Fix $\gamma > 0$. For any tree or half-tree T, define $\tilde{n} = \tilde{n}(T)$ to be $\tilde{n} = (n - n_1) + \gamma n_1$, where n is the number of vertices of T and n_1 the number of degree 1 vertices (leaves) of T. In other words, $\tilde{n}$ is the number of vertices of T but with each leaf counting as γ vertices.

For any tree or half-tree T, and any $\alpha, \beta, \gamma > 0$, define

$$c_T = c_T(\alpha, \beta, \gamma) = R_{-\alpha}(T) - \beta\tilde{n}(T). \tag{1}$$

If T is a non-trivial half-tree composed of half-trees $T_1, \ldots T_{d(v_0)-1}$ joined via their dangling edges to the root v_0 of T, then

$$c_T = \sum_{i=1}^{d(v_0)-1} (c_{T_i} + (d(v_0)d(v_i))^{-\alpha}) - \beta, \tag{2}$$

where v_i is the root of T_i. Also, if T is a tree obtained by joining two half-trees T_1 and T_2 (with roots v_1, v_2) via their dangling edges, then

$$c_T = c_{T_1} + c_{T_2} + (d(v_1)d(v_2))^{-\alpha}. \tag{3}$$

For any finite sequence of integers $a_0, a_1, \ldots, a_r$ with $a_r = 1$ and $a_i > 1$ for $i < r$, define a half-tree $[a_0, \ldots, a_r]$ by inductively attaching $a_0 - 1$ copies of $[a_1, \ldots, a_r]$ (via their dangling edges) and one dangling edge to a vertex v_0 (see Figure 1). Alternatively, it is the unique half-tree such that all vertices at distance i from v_0 have degree a_i.

It is easy to determine $c_T(\alpha, \beta, \gamma)$ for half-trees of the form $[a_0, \ldots, a_r]$. As we will see later in Lemma 4, for the values of β we are interested in, and for $d \geq 2$, there is a half-tree $[a_0, \ldots, a_r]$ with $d = a_0 > a_1 > \cdots > a_r = 1$ that maximizes c_T over all half-trees with $d(v_0) = d$. Thus it is sufficient to find an upper bound on c_T for all half-trees of this form. To do so, fix $\alpha, \beta, \gamma > 0$. Define $c_d = c_d(\alpha, \beta, \gamma)$ inductively by

$$c_1 = -\gamma\beta \tag{4}$$

and for $d \geq 2$,

$$c_d = (d - 1) \max_{1 \leq k < d} \{c_k + (kd)^{-\alpha}\} - \beta. \tag{5}$$

Thus the first few values of c_d are

$$\begin{aligned} c_1 &= -\gamma\beta, \\ c_2 &= 2^{-\alpha} - (1+\gamma)\beta, \\ c_3 &= 2\ \max\{3^{-\alpha}, 2^{-\alpha} - \beta + 6^{-\alpha}\} - (1+2\gamma)\beta. \end{aligned}$$

The next lemma shows that c_d is an upper bound on c_T over all half-trees T of the form $T = [a_0, \ldots, a_r]$ with $d = a_0 > a_1 > \cdots > a_r = 1$.

Lemma 1. *The constant $c_d = c_d(\alpha, \beta, \gamma)$ is the maximum value of $c_T(\alpha, \beta, \gamma)$ over all half-trees of the form $T = [a_0, \ldots, a_r]$ where $d = a_0 > a_1 > \cdots > a_r = 1$.*

Proof. The result clearly holds for $d = 1$, since then T is the trivial half-tree and thus $c_T = -\gamma\beta = c_1$. For $d = a_0 > 1$, (2) gives $c_T = (a_0 - 1)(c_{T'} + (a_0 a_1)^{-\alpha}) - \beta$ where $T' = [a_1, \ldots, a_r]$. By induction on d, this is maximal (for fixed a_1) when $c_{T'} = c_{a_1}$. Maximizing over a_1, $1 \le a_1 < a_0$, gives $c_T = c_{a_0} = c_d$ by (5). □

Define $\beta_c = \beta_c(\alpha, \gamma)$ to be the infimum of all $\beta > 0$ such that for all $d \ge 2$,

$$c_d \ge (d-1)(c_d + d^{-2\alpha}) - \beta. \tag{6}$$

In other words (5) still holds if we extend the maximum to include $k = d$. We shall show now that β_c exists. Note that condition (6) is equivalent to

$$\beta \ge 4^{-\alpha}, \tag{7}$$

for $d = 2$, and to

$$c_d \le \frac{\beta - d^{-2\alpha}(d-1)}{(d-2)} \tag{8}$$

for $d > 2$. If $\beta = \max\{1/\gamma, 1\}$ then by (4), (5) and induction on d one can show that $c_d \le -1$ for all $d \ge 1$. Thus for this value of β, (7), (8), and hence (6) are satisfied. Now c_d is a strictly decreasing function of β for all $d \ge 1$. Thus β_c exists and

$$4^{-\alpha} \le \beta_c \le \max\{1/\gamma, 1\}. \tag{9}$$

For $\gamma = 1$, the function β_c is plotted as a function of α in Figure 2.

Note that for each $d \ge 1$ the function c_d is decreasing and continuous (piecewise linear) in β and so in particular the following observation is true.

Observation 2. *If $\beta \ge \beta_c$, then* (8) *is satisfied for all $d > 2$, and* (6) *is satisfied for all $d \ge 2$.*

If condition (6) holds for all $d \ge 2$ (so in particular if $\beta \ge \beta_c$) then for all $d \ge 1$

$$c_d \le 0, \tag{10}$$

as otherwise (5) implies that, for N sufficiently large, $c_N > (N-1)c_d - \beta > \frac{\beta}{N-2}$ contradicting (8) and thus contradicting (6).

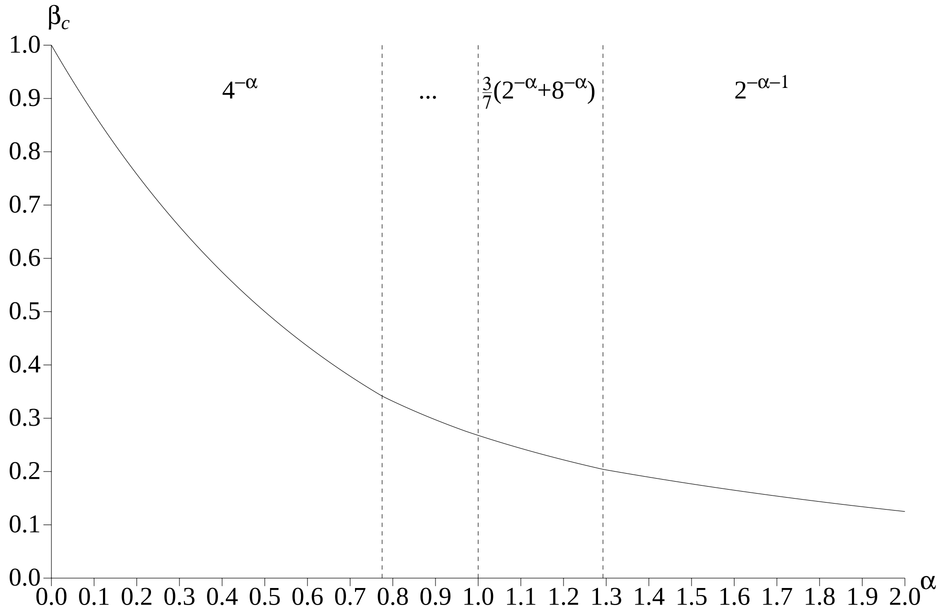

Figure 2: The function $\beta_c = \beta_c(\alpha, \gamma)$ for $\gamma = 1$.

3 The upper bound

In this section we shall show that $\beta_c = \beta_c(\alpha, \gamma)$ as defined in the previous section is the constant we are looking for, that is, $R_{-\alpha}(T) \leq \beta_c(\tilde{n}+1)$ for all trees T on at least 3 vertices.

Lemma 3. *If $\beta \geq \beta_c$ then $c_d \geq (d-1)(c_k + (kd)^{-\alpha}) - \beta$ for all $d \geq 2$ and $k \geq 1$.*

Proof. Fix $\beta \geq \beta_c$ and assume for contradiction that the result is false. Take a minimal d, and then a minimal k that gives a counterexample. By the definition of c_d (see (5)) we may assume $k \geq d$, and by Observation 2 and (6) we may assume $k \neq d$. Thus $k > d$. Now, by our assumption, we have

$$c_d < (d-1)(c_k + (kd)^{-\alpha}) - \beta.$$

But, by our choice of k, we have

$$c_d \geq (d-1)(c_t + (td)^{-\alpha}) - \beta$$

for all t with $1 \leq t < k$. Thus

$$c_t + t^{-\alpha}d^{-\alpha} < c_k + k^{-\alpha}d^{-\alpha}.$$

But $\alpha > 0$, so $t^{-\alpha} > k^{-\alpha}$ and $d^{-\alpha} > k^{-\alpha}$. Thus

$$c_t + t^{-\alpha}k^{-\alpha} < c_k + k^{-\alpha}k^{-\alpha}$$

for all t with $1 \le t < k$. But then

$$c_k = (k-1)\max_{1\le t<k}(c_t + (tk)^{-\alpha}) - \beta < (k-1)(c_k + k^{-2\alpha}) - \beta$$

contradicting (6). □

Lemma 4. *If $\beta \ge \beta_c$, then $c_T \le c_d$ for any half-tree T with root v_0 of degree d.*

Proof. We prove the result by induction on the depth of the half-tree. If the half-tree is trivial, then $R_{-\alpha}(T) = 0$ and $c_T = -\gamma\beta = c_1$ (note that v_0 has degree 1 due to the dangling edge). Now assume the result holds for all half-trees of smaller depth. In particular, if we consider T to be formed by joining half-trees $T_1, \dots, T_{d-1}$ to v_0, then $c_{T_i} \le c_{d(v_i)}$ where the half-tree T_i has root v_i. Thus by (2)

$$\begin{aligned} c_T &= \sum_{i=1}^{d-1}(c_{T_i} + (dd(v_i))^{-\alpha}) - \beta \\ &\le \sum_{i=1}^{d-1}(c_{d(v_i)} + (dd(v_i))^{-\alpha}) - \beta \\ &\le (d-1)\sup_{k\ge1}(c_k + (dk)^{-\alpha}) - \beta. \end{aligned}$$

But as the root of any non-trivial half-tree has degree at least 2, it follows from Lemma 3 that $(d-1)\sup_{k\ge1}(c_k + (dk)^{-\alpha}) - \beta \le c_d$, so $c_T \le c_d$. □

As we have just seen, c_d is an upper bound on c_T for all half-trees and all $\beta \ge \beta_c$. In the following theorem we use this result to prove an upper bound on c_T for trees.

Theorem 5. *For any $\alpha, \gamma > 0$ and any tree T with $n = |V(T)| \ge 3$,*

$$R_{-\alpha}(T) \le \beta_c(\tilde{n} + 1) = \beta_c((n - n_1) + \gamma n_1 + 1),$$

where as before $\beta_c = \beta_c(\alpha, \gamma)$ is the infimum of all β satisfying (6) for all $d \ge 2$ and n_1 is the number of leaves of T.

Proof. Let Δ be the maximum degree of T and fix $\beta = \beta_c$. Since $n \ge 3$, we have $\Delta \ge 2$. Let uv be an edge of T with $d(u) = \Delta$ and $d(v) = k \le \Delta$. It follows from (3) and Lemma 4 that $c_T \le c_\Delta + c_k + (k\Delta)^{-\alpha}$. By Lemma 3,

$$c_\Delta \ge (\Delta - 1)(c_k + (k\Delta)^{-\alpha}) - \beta_c,$$

which implies $c_k + (k\Delta)^{-\alpha} \le (\beta_c + c_\Delta)/(\Delta - 1)$. (Indeed, by the definition of c_Δ there exists a $k < \Delta$ which achieves equality.) Thus $c_T \le (\beta_c + \Delta c_\Delta)/(\Delta - 1)$. Now by (10) we have $c_\Delta \le 0$. Hence $c_T \le \beta_c/(\Delta - 1)$ and

$$R_{-\alpha}(T) = \beta_c\tilde{n} + c_T \le \beta_c\left(\tilde{n} + \tfrac{1}{\Delta-1}\right) \le \beta_c(\tilde{n} + 1).$$

□

With essentially the same proof one can show the following theorem.

Theorem 6. *For any $\alpha, \gamma > 0$ and for any tree T with maximum degree $\Delta > 1$,*

$$R_{-\alpha}(T) \leq \beta_\Delta \tilde{n} + \tfrac{1}{\Delta-1}(\beta_\Delta + \Delta c_\Delta(\alpha, \beta_\Delta, \gamma)),$$

where $\beta_\Delta = \beta_\Delta(\alpha, \gamma)$ is the minimum of all β such that (6) is satisfied for all $2 \leq d \leq \Delta$. □

For example if $\alpha = \gamma = 1$ then any tree T with maximum degree 3 satisfies $R_{-1}(T) \leq \frac{7}{27}n + \frac{5}{27}$ as at $\beta = \frac{7}{27} \geq 4^{-\alpha}$, we have $c_1 = -\frac{7}{27}$, $c_2 = -\frac{1}{54}$ and $c_3 = \frac{1}{27}$, giving equality in (8) at $d = 3$. Note that when we restrict the maximum degree then (10) need not hold. For more precise results in this special case see [10]. If $\alpha = \gamma = 1$, then any tree T with maximum degree 4 (a chemical tree) satisfies $R_{-1}(T) \leq \frac{139}{528}n + \frac{73}{528}$; see also [5].

Note that the additive constant in Theorems 5 and 6 can be made sharp for any given α and γ simply by finding the values of c_Δ. Indeed, the proof of Theorem 5 shows that

$$R_{-\alpha}(T) \leq \beta_c \tilde{n} + \tfrac{\beta_c + \Delta c_\Delta}{\Delta - 1}, \tag{11}$$

and Lemma 1 shows that there is a half-tree $T' = [\Delta, k, \dots, 1]$ with $c_{T'} = c_\Delta$. But then the tree T obtained by joining $[\Delta, k, \dots, 1]$ to $[k, \dots, 1]$ (equivalently Δ copies of $[k, \dots, 1]$ joined to a single vertex) has $c_T = \frac{\beta_c + \Delta c_\Delta}{\Delta - 1}$ and thus its Randić index is exactly $\beta_c \tilde{n} + \frac{\beta_c + \Delta c_\Delta}{\Delta - 1}$.

4 Many trees with large Randić index

To exhibit infinitely many trees T with $R_{-\alpha}(T) \geq \beta_c(\tilde{n} - 1)$, we first show that if c_d is sufficiently large and negative then (6) is satisfied for all larger d as well.

Lemma 7. *Let $\beta \geq 4^{-\alpha}$. If $c_t = c_t(\alpha, \beta, \gamma) \leq -\beta$ for some $t \geq 2$ then, for all $d > t$, $c_d(\alpha, \beta, \gamma) < -\beta$. In particular, if $d > t$ then (6) is satisfied with strict inequality.*

Proof. We first show that $c_{t+1}(\alpha, \beta, \gamma) < -\beta$. By the definition (5) of c_t and since $c_t \leq -\beta$, we have $c_k + (kt)^{-\alpha} \leq 0$ for all $1 \leq k < t$ and thus

$$c_k + (k(t+1))^{-\alpha} < c_k + (kt)^{-\alpha} \leq 0.$$

But as $\beta \geq 4^{-\alpha}$ and $t \geq 2$

$$c_t + (t(t+1))^{-\alpha} < c_t + \beta \leq 0.$$

Thus, by the definition of c_{t+1}, we have $c_{t+1} < -\beta$. Now, by induction on d, $c_d < -\beta$ for all $d > t$. If $d > t \geq 2$ then $\beta \geq 4^{-\alpha} > d^{-2\alpha}$, so

$$\frac{\beta - d^{-2\alpha}(d-1)}{d-2} > \frac{\beta - \beta(d-1)}{d-2} = -\beta > c_d.$$

Thus (8) is satisfied with strict inequality, which is equivalent to (6) being satisfied with strict inequality. □

Let $\beta \geq 4^{-\alpha}$. If $\gamma \geq 2^{\alpha}$ then $c_2 = 2^{-\alpha} - (1+\gamma)\beta \leq -\beta$. Hence by Lemma 7, (6) is satisfied for all $d \geq 2$ and thus the following proposition is true.

Proposition 8. *If* $\gamma \geq 2^{\alpha}$ *then* $\beta_c(\alpha, \gamma) = 4^{-\alpha}$.

Let $\beta = \beta_c$ and define $d_c = d_c(\alpha, \gamma)$ to be the smallest d that gives equality in (6). We set $d_c = \infty$ if no such d exists. In particular, if $d_c < \infty$, then

$$c_{d_c}(\alpha, \beta_c, \gamma) = (d_c - 1)(c_{d_c}(\alpha, \beta_c, \gamma) + d_c^{-2\alpha}) - \beta_c.$$

Lemma 9. *If* $d_c(\alpha, \gamma) = d_c > 2$ *then for all* d *with* $2 \leq d \leq d_c$ *we have* $c_d(\alpha, \beta_c, \gamma) \geq -\beta_c$.

Proof. Assume first that $d_c < \infty$. By (9), we have $\beta_c \geq 4^{-\alpha} \geq d_c^{-2\alpha}$, and hence as $d_c > 2$, equality in (6) implies

$$c_{d_c}(\alpha, \beta_c, \gamma) = \frac{\beta_c - d_c^{-2\alpha}(d_c - 1)}{d_c - 2} \geq \frac{\beta_c - \beta_c(d_c - 1)}{d_c - 2} = -\beta_c.$$

In particular, the statement of the lemma is true for $d = d_c$.

Now assume that $c_d(\alpha, \beta_c, \gamma) < -\beta_c$ for some d, $2 \leq d < d_c \leq \infty$. Then by continuity of c_d there exists a β' with $\beta' < \beta_c$ and $c'_d = c_d(\alpha, \beta', \gamma) < -\beta'$. Since $d < d_c$, we may also assume that (6) holds for $\beta = \beta'$ and all k, $2 \leq k \leq d$, and thus in particular $\beta' \geq 4^{-\alpha}$. For $k \geq d$, it follows from Lemma 7 that (6) is satisfied for $c_k(\alpha, \beta', \gamma)$. Therefore (6) is satisfied for all $k \geq 2$ at β'. But then $\beta_c \leq \beta'$ — a contradiction. Thus $c_d(\alpha, \beta_c, \gamma) \geq -\beta_c$ for all d, $2 \leq d \leq d_c$. □

Theorem 10. *For* $0 < \gamma \leq 2^{\alpha}$, *there exist infinitely many trees* T *with* $R_{-\alpha}(T) \geq \beta_c(\tilde{n}-1)$.

Proof. Let $\beta = \beta_c(\alpha, \gamma)$. By Lemma 1, we can, for all d, fix a half-tree T_d of the form $[a_0, \ldots, a_r]$ with $d = a_0 > a_1 > \cdots > a_r = 1$ and $c_{T_d} = c_d$. For $d \geq 2$, consider the tree T'_d which consists of d half-trees $[a_1, \ldots, a_r]$ and a vertex v such that the dangling edges of the half-trees are joined to v. Then $c_{T'_d} = d(c_{a_1} + (da_1)^{-\alpha}) - \beta_c = \frac{d}{d-1}(c_d + \beta_c) - \beta_c$.

If $d_c = \infty$ then we obtain infinitely many trees by considering T'_d for infinitely many values of $d > 2$. Indeed, by Lemma 9, $c_d \geq -\beta_c$, so $c_{T'_d} \geq -\beta_c$ and $R_{-\alpha}(T'_d) = \beta_c\tilde{n} + c_{T'_d} \geq \beta_c(\tilde{n}-1)$.

If $d_c < \infty$, write $T_{d_c} = [d_c, a_1, \ldots, a_r]$ as before. Let $T_{(i)} = [d_c, d_c, \ldots, d_c, a_1, \ldots, a_r]$ where d_c is repeated i times. By (2) and the definition of d_c we have $c_{T_{(i)}} = c_{T_{d_c}} = c_{d_c}$. For each i construct $T'_{(i)}$ by joining d_c copies of $T_{(i)}$ to a single vertex v. Then as before, $c_{T'_{(i)}} = \frac{d_c}{d_c-1}(c_{d_c} + \beta_c) - \beta_c$. For $d_c > 2$, Lemma 9 implies $c_{d_c} \geq -\beta_c$ and hence $c_{T'_{(i)}} \geq -\beta_c$. Therefore we have infinitely many trees T such that $R_{-\alpha}(T) = \beta_c\tilde{n} + c_T \geq \beta_c(\tilde{n} - 1)$.

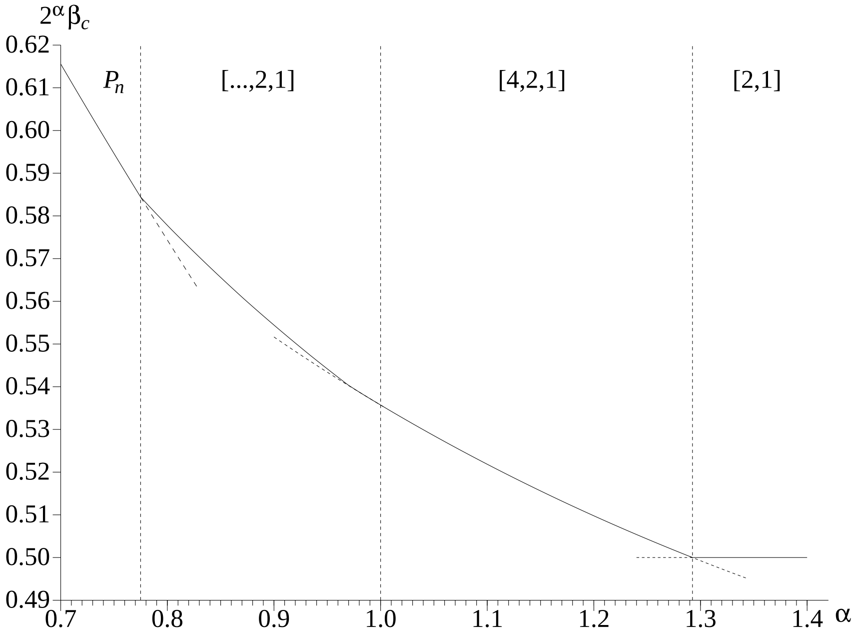

Figure 3: The function β_c scaled by 2^α in the region $0.7 < \alpha < 1.4$ for $\gamma = 1$ together with optimal half-trees.

If $d_c = 2$, then $\beta_c = 4^{-\alpha}$ and $T = T'_{(i)}$ is a path. Hence

$$\begin{aligned} R_{-\alpha}(T) &= 4^{-\alpha}(n-3) + 2^{-\alpha} \cdot 2 \\ &\geq 4^{-\alpha}(\tilde{n}-1) - 2\gamma 4^{-\alpha} + 2^{-\alpha+1} \\ &\geq 4^{-\alpha}(\tilde{n}-1), \end{aligned}$$

as $\gamma \leq 2^\alpha$. □

We saw in Proposition 8 that if $\gamma \geq 2^\alpha$ then $\beta_c = 4^{-\alpha}$ and the family of paths shows that one cannot improve β_c, but the additive constant is worse than $4^{-\alpha}$. Let us consider the shape of some of the trees or half-trees encountered in the proof of Theorem 10. If $d_c < \infty$ then the maximal value of c_T is achieved by half-trees of the form $[d_c, d_c, \ldots, d_c, a_1, a_2, \ldots, 1]$. Thus the Randić index is maximal (or close to maximal) for trees consisting of a large d_c-regular part with half-trees $[a_1, \ldots, 1]$ attached to the 'outside' vertices. As a special case, if $d_c = 2$ then these trees are paths. If $d_c = \infty$ then for large n the optimal tree must have a high degree vertex (since $\beta_\Delta < \beta_c$ when $\Delta < d_c$). As we shall see later in Section 5, if $\alpha \geq 1$ then this high degree vertex will be joined to half-trees $[d, k, \ldots, 1]$ with $c_d = 0$, $k \in \{1, 2, 3\}$. Thus the tree will have bounded diameter. If $\alpha < 1$ then the high degree vertex will be joined to other vertices which also have high degree, but not so high. In this case we obtain half-trees that look like $[\ldots, b_2, b_1, 1]$ where $1 < b_1 < b_2 < b_3 < \ldots$. Figure 4 shows the optimal half-trees as a function of α and γ.

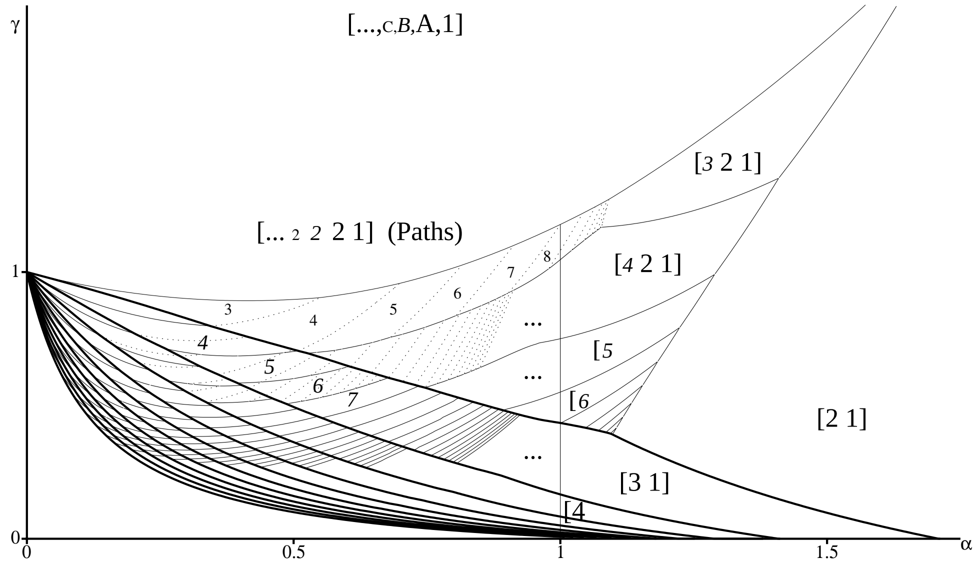

Figure 4: Optimal half-trees in the form $[\ldots, C, B, A, 1]$ for different α and γ. Regions with different values of A (respectively B, C) are separated by thick lines (respectively thin lines, dotted lines). Above the top curve, the optimal half-trees are paths $[2, \ldots, 2, 1]$. For $\alpha \geq 1$ and below the top curve, the optimal half-trees are of bounded diameter.

As for the upper bound there exists a corresponding result to Theorem 10 for trees with bounded maximum degree.

Theorem 11. *For $0 < \gamma \leq 2^\alpha$, there are infinitely many trees T with maximum degree at most $\Delta > 1$ such that*

$$R_\alpha(T) \geq \beta_\Delta(\tilde{n} - 1),$$

where $\beta_\Delta = \beta_\Delta(\alpha, \gamma)$ is the minimum of all β such that (6) is satisfied for all $2 \leq d \leq \Delta$. □

For fixed α the trees encountered in Theorem 10 vary. As an example, consider the case $\alpha = 1$. As γ decreases, the number of leaves in the optimal half-tree (which has $c_T = 0$) increases (see Figure 5). The maximal Randić index occurs with $[4, 2, 1]$, but if we wish to restrict the fraction of leaves (by varying γ), then we get other trees. We conclude this section with the following theorem that states that these trees are essentially best possible if we are interested in trees with a certain fraction of leaves.

Theorem 12. *For each fixed $\alpha > 0$ and each $x_0 \in [0, 1)$, there exists an infinite sequence of trees T_k with $n_1(T_k)/n(T_k) \to x_0$ and $R_{-\alpha}(T_k) = \inf_{\gamma>0} \beta_c(\alpha, \gamma)\tilde{n} + o(n)$ as $k \to \infty$.*

Proof. Consider the set C_α of all points $(a, b) \in \mathbb{R}^2$ such that there exists an infinite sequence of trees $T_1, T_2, \ldots$ such that $n_1(T_i)/n(T_i) \to a$ and $R_{-\alpha}(T_i)/n(T_i) \to b$ as $i \to \infty$. We call the points of C_α *relevant.* Thus the set C_α is the set of accumulation points of the set of pairs $(n_1(T)/n(T), R_{-\alpha}(T)/n(T))$, where T runs over the set of all trees. As a consequence,

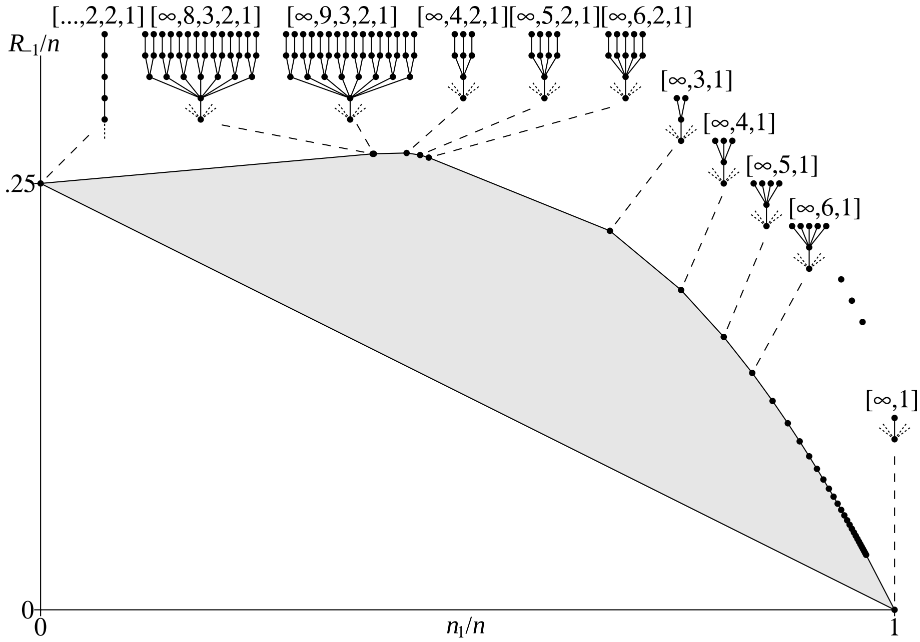

Figure 5: The set C_α of relevant points and the progression of optimal trees with increasing number of leaves for $\alpha = 1$. The lower boundary follows from Theorem 5 of [7]. We denote by $[\infty, d, k, \ldots, 1]$ trees obtained by joining a high degree vertex to many copies of $[d, k, \ldots, 1]$.

C_α is a closed subset of $\mathbb{R}^2$. For $\gamma > 0$, let $l_\gamma(x) = \beta_c(\alpha, \gamma) + \beta_c(\alpha, \gamma)(\gamma - 1)x$. Note that by Theorem 5 the set C_α lies below the line $y = l_\gamma(x)$ for all $\gamma > 0$. In fact we shall show that the lines $l_\gamma(x)$ determine the upper boundary of C_α. First note that by Theorem 10 there is at least one relevant point on each line $l_\gamma(x)$. Indeed, there are infinitely many trees T with $R_{-\alpha}(T)/n(T) \geq \beta_c + \beta_c(\gamma - 1)n_1(T)/n(T) - \beta_c/n(T)$ and as $n_1(T)/n(T) \in [0, 1]$ there must be an $a \in [0, 1]$ and an infinite (sub-)sequence $T_1, T_2, \ldots$ of these trees with $n_1(T_i)/n(T_i) \to a$ as $i \to \infty$. We claim that for each fixed $\alpha > 0$, the set C_α of relevant points is convex. To prove the claim let (a, b) and (a', b') be two relevant points. Consider an infinite sequence of trees $T_1, T_2, \ldots$ certifying that (a, b) is a relevant point, and an infinite sequence of trees $T_1', T_2', \ldots$ certifying that (a', b') is a relevant point. Fix $\mu \in (0, 1)$. Construct trees $\tilde{T}_i$ by taking $N' = \lceil \mu n(T_i) \rceil$ copies of T_i', $N = \lceil (1 - \mu)n(T_i') \rceil$ copies of T_i, and an extra vertex that is adjacent to a (non-leaf) vertex from each of these $N + N'$ trees. Then

$$\frac{n(\tilde{T}_i)}{n(T_i)n(T_i')} = \frac{Nn(T_i) + N'n(T_i') + 1}{n(T_i)n(T_i')} \to (1 - \mu) + \mu = 1, \tag{12}$$

and

$$\frac{n_1(\tilde{T}_i)}{n(T_i)n(T_i')} = \frac{Nn_1(T_i) + N'n_1(T_i')}{n(T_i)n(T_i')} \to (1 - \mu)a + \mu a', \tag{13}$$

as $i \to \infty$. Adding a dangling edge to a vertex of degree d of T_i decreases its Randić index by at most $d(d^{-\alpha} - (d + 1)^{-\alpha}) \leq \alpha d^{-\alpha} \leq \alpha$, and adding a new vertex of degree d increases the Randić index by at most $d(d)^{-\alpha} \le d$. Thus

$$NR_{-\alpha}(T_i) + N'R_{-\alpha}(T_i') - (N+N')\alpha \le R_{-\alpha}(\tilde{T}_i) \le NR_{-\alpha}(T_i) + N'R_{-\alpha}(T_i') + (N+N').$$

Therefore

$$\frac{R_{-\alpha}(\tilde{T}_i)}{n(T_i)n(T_i')} \to (1-\mu)b + \mu b' \tag{14}$$

as $i \to \infty$. Combining (12)–(14) we see that

$$\left(\tfrac{n_1(\tilde{T}_i)}{n(\tilde{T}_i)}, \tfrac{R_{-\alpha}(\tilde{T}_i)}{n(\tilde{T}_i)}\right) \to ((1-\mu)a + \mu a', (1-\mu)b + \mu b') \qquad \text{as } i \to \infty,$$

so the point $((1-\mu)a+\mu a', (1-\mu)b+\mu b')$ is relevant. This proves that the set C_α of relevant points is convex.

Next we show that $\beta_c(\alpha,\gamma)$ is continuous in γ. On each line $y = l_\gamma(x)$ there is a relevant point and no relevant point can lie above any line $y = l_\gamma(x)$. It follows that any two of these lines must intersect in $[0,1]$. Fix $\gamma > 0$ and $\gamma' > 0$. Let $\beta = \beta_c(\alpha,\gamma)$ and $\beta' = \beta_c(\alpha,\gamma')$. Suppose that $l_\gamma(0) = \beta$ lies below $l_{\gamma'}(0) = \beta'$. Since l_γ and $l_{\gamma'}$ cross in $[0,1]$, $\gamma\beta = l_\gamma(1) \ge l_{\gamma'}(1) = \gamma'\beta'$. Hence $\beta < \beta' \le \beta\gamma/\gamma'$. Similarly, if β' lies below β then $\gamma\beta \le \gamma'\beta'$ so $\beta\gamma/\gamma' \le \beta' < \beta$. Thus in general

$$\min(\gamma/\gamma', 1)\beta \le \beta' \le \max(\gamma/\gamma', 1)\beta.$$

Thus if $\gamma' \to \gamma > 0$ then $\beta' \to \beta$. Hence $\beta_c(\alpha,\gamma)$ is a continuous function of γ.

Now we can show that the lines l_γ define the upper boundary of the set C_α. We note that the extremal values of $n_1(T)/n(T)$ occur for paths, giving the relevant point $P_0 = (0, 4^{-\alpha})$, and stars, giving the relevant point $P_1 = (1,0)$. For $\gamma \ge 2^\alpha$, $\beta_c = 4^{-\alpha}$ and so P_0 lies on l_γ. For $\gamma < 1$, $l_\gamma(1/(1-\gamma)) = 0$, but as $\gamma \to 0$, $1/(1-\gamma) \to 1$. thus P_1 is a limit of points on the lines l_γ. Now fix $x_0 \in [0,1)$. Let (x_0, y) be a point on the upper boundary of C_α. Since C_α is closed, $(x_0,y) \in C_\alpha$ and hence (x_0,y) is relevant. However, C_α is convex, so there is a line through (x_0,y) lying above C_α. Moreover, the slope of the line must lie between the slopes of the lines corresponding to P_0 and P_1. But by continuity of β_c, this line must now occur as some l_γ or as a limit of the lines l_γ as $\gamma \to 0$. The result follows. □

Let us remark that for $\alpha \le 1$ the infimum in the statement of the previous theorem is attained at some $\gamma > 0$. To see this note that

$$0 \ge c_c \ge (d-1)(c_1 + d^{-\alpha}) - \beta = (d-1)(-\gamma\beta + d^{-\alpha}) - \beta$$

and thus $\beta \ge d^{-\alpha}(d-1)/(1+(d-1)\gamma)$. Hence if $\alpha < 1$ and $\gamma \to 0$ then $\beta = \beta(\alpha,\gamma) \to \infty$ and therefore

$$\beta\tilde{n} = \beta(n - (1-\gamma)n_1) = \beta(1 - x_0 + \gamma x_0 + o(1))n \to \infty$$

as x_0 is less than 1. If $\alpha = 1$, then we can use Proposition 13 to deduce that for sufficiently small γ, $\beta = \max_{d\ge 2}(d-1)/((1+(d-1)\gamma)d)$ and that $c_{T_d} = 0$ for the half-tree $T_d = [d,1]$

where $d = d(\gamma)$ achieves the maximum in the formula for β; see Figure 5. As $d \to \infty$ as $\gamma \to 0$, it follows that $n_1(T_d)/n(T_d) \to 1$ as $\gamma \to 0$. Thus for sufficiently small $\gamma > 0$, the line l_γ meets C_α to the right of $x = x_0$ and therefore by continuity of the slopes there exists a $\gamma > 0$ such that l_γ meets C_α at $x = x_0$.

5 Calculating β_c

It is easy to calculate β_c with the following straightforward algorithm. Fix $\alpha > 0$ and $\gamma > 0$. Pick some $\beta > 0$ and calculate c_d inductively using the definition (5). As we have already observed c_d is a decreasing function of β. Moreover, the derivative of c_d with respect to β is at least $(d-1)+\gamma$ (and is usually much larger). For each d in turn one can check condition (6). If (6) fails then $\beta < \beta_c$. If $c_d > 0$ then once again $\beta < \beta_c$. However, if $c_d \leq -\beta$ and (6) held (with strict inequality) for all values of d so far, then by Lemma 9 $\beta > \beta_c$. Thus we see that if c_d ever leaves the interval $[-\beta, 0]$ then we will have determined whether β is less than or greater than β_c. On the other hand, since the derivative of c_d with respect to β grows with d, the interval of possible values for β for which the algorithm has not decided by d whether $\beta < \beta_c$ or $\beta > \beta_c$ must be small. Thus β_c can be calculated to any desired accuracy.

The following results help in calculating β_c.

Proposition 13. *If $\alpha \geq 1$, then β_c is the minimum over all β satisfying*

$$\beta \geq 4^{-\alpha} \quad \text{and} \quad (d-1)(c_k(\alpha,\beta,\gamma) + (kd)^{-\alpha}) \leq \beta \tag{15}$$

for $k \in \{1,2,3\}$ and all integers $d > k$. Moreover, either $\beta = 4^{-\alpha}$ or $c_d = 0$ for some $d \geq 2$.

Proof. Let β be such that conditions (15) are satisfied. We first show that $c_d(\alpha,\beta,\gamma) \leq 0$ for all d. Note first that (15) implies that $c_1, c_2, c_3 \leq 0$. Let $d \geq 4$ and assume that $c_k \leq 0$ for all $1 \leq k < d$. Then by the definition of c_d there exists a $1 \leq k < d$ such that $c_d = (d-1)(c_k + (kd)^{-\alpha}) - \beta$. If $k \leq 3$ then (15) implies that $c_d \leq 0$. If $k \geq 4$ then $(d-1)(kd)^{-\alpha} \leq 4^{-\alpha} \leq \beta$ and thus $c_d \leq (d-1)c_k \leq 0$.

To see that (6) is satisfied for all $d \geq 2$, note that (6) is satisfied for $d = 2$ as $\beta \geq 4^{-\alpha}$. For $d \geq 3$, $d^{-2\alpha}(d-1) \leq 2/9^\alpha \leq 4^{-\alpha} \leq \beta$ and thus (8) is satisfied as $c_d(\alpha,\beta,\gamma) \leq 0$. But for $d \geq 3$ (8) is equivalent to (6). Thus $\beta_c \leq \beta$ for any β satisfying (15). It is easily verified that β_c satisfies (15) and the first claim follows.

Finally, if $c_1, c_2, c_3 < 0$, then (15) automatically holds for all sufficiently large d. Thus we only have to check a finite number of conditions. Thus at $\beta = \beta_c$ one of the inequalities in (15) must be an equality. But then either $\beta = 4^{-\alpha}$ or some $c_d = 0$. □

Let us calculate $\beta_c(1,1)$. We have $c_1 = -\beta$ and $c_2 = 2^{-1} - 2\beta$. Using condition (15) with $k = 2$, we know that β_c has to satisfy that for all $d \geq 3$,

$$(d-1)(2^{-1} - 2\beta_c + (2d)^{-1}) - \beta_c \leq 0,$$

or equivalently,

$$\beta_c \geq \frac{d^2 - 1}{2d(2d-1)}.$$

It is easily seen that the right-hand side of the last equation is maximized when $d = 4$ and thus $\beta_c(1,1) \geq \frac{15}{56}$. Now $c_3(1, \frac{15}{56}, 1) = -\frac{1}{168}$ and one can verify that

$$(d-1)(-\tfrac{1}{168} + (3d)^{-1}) \leq \tfrac{15}{56},$$

for all $d \geq 4$. As $\frac{15}{56} \geq 4^{-1}$ conditions (15) are satisfied and thus $\beta_c(1,1) = \frac{15}{56}$. It follows from Theorem 5 that for all trees on at least 3 vertices $R_{-1}(T) \leq \frac{15}{56}|V(T)| + \frac{15}{56}$, which slightly improves the result in [4].

In contrast to Proposition 13 we have the following.

Proposition 14. *If $0 < \alpha < 1$ and $\beta \geq \beta_c$ then $c_d(\alpha, \beta, \gamma) < 0$ for all $d \geq 1$. Moreover if $d_c = d_c(\alpha, \gamma) = \infty$ then the value of k that achieves the maximum in* (5) *tends to ∞ as $d \to \infty$.*

Proof. If $c_k \geq 0$ then by (5) $c_d \geq (d-1)(dk)^{-\alpha} - \beta$ is positive for sufficiently large d, contradicting (10). Thus $c_k < 0$ and for sufficiently large d, $(d-1)(c_k + (kd)^{-\alpha}) < 0$. But by Lemma 9, $c_d > -\beta$. Hence k cannot achieve the minimum in (5) for c_d. □

Proposition 15. *If $0 < \alpha < 1/2$ then $d_c(\alpha, \gamma) < \infty$, that is, condition* (6) *is satisfied with equality for some d.*

Proof. Assume that $d_c(\alpha, \gamma) = \infty$. If we had a uniform bound $c_k \leq -c < 0$ for all $k \geq 1$, then for sufficiently large d, we would have $c_k + (kd)^{-\alpha} < 0$ for all k and so $c_d < -\beta$ contradicting Lemma 9. Thus $\limsup_{k\to\infty} c_k = 0$. But by Proposition 14 $c_k < 0$ for all $k \geq 1$. Thus there must be a sequence of d's such that c_d is larger than all previous c_d's. Take such a suitably large d and define k so that

$$c_d = (d-1)(c_k + (kd)^{-\alpha}) - \beta.$$

By Proposition 14 we may choose d in such a way that k is arbitrarily large. Now by our choice of d and k,

$$(d-1)(c_k + (kd)^{-\alpha}) - \beta = c_d > c_k \geq (k-1)(c_k + k^{-2\alpha}) - \beta.$$

Simplifying gives

$$(d-k)c_k > (k-1)k^{-2\alpha} - (d-1)(kd)^{-\alpha}.$$

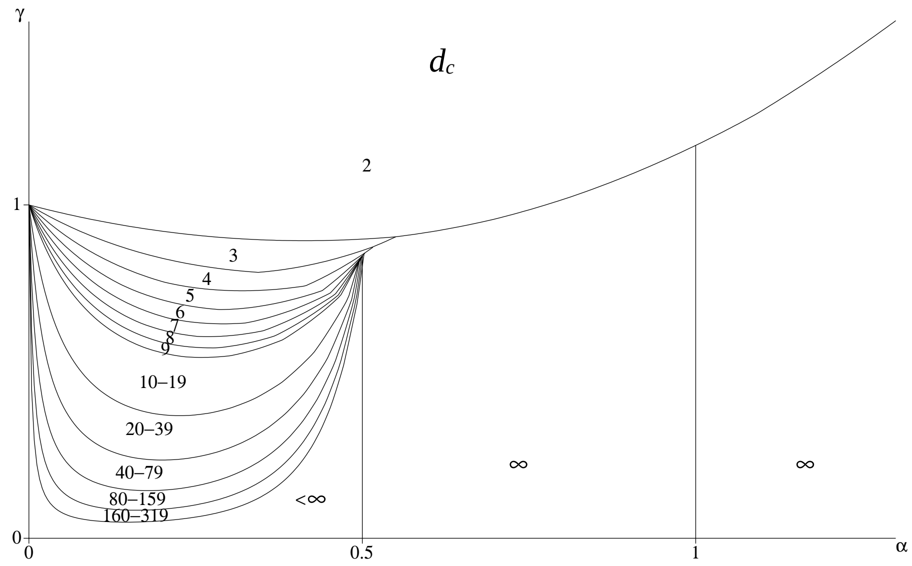

Figure 6: The value of d_c as a function of α and γ.

Note that for $d = k$ this is an equality, so by differentiating both sides with respect to d, there must be some real x, $k < x < d$ such that

$$c_k > (\alpha(x-1)/x-1)(kx)^{-\alpha}.$$

Since $x > k \geq 2$, we must have

$$c_k > (\alpha/2-1)k^{-2\alpha}.$$

But by (6)

$$(k-2)c_k \leq \beta + (k-1)k^{-2\alpha},$$

so

$$(\alpha/2-1)(k-2)k^{-2\alpha} < \beta + (k-1)k^{-2\alpha},$$

or, equivalently,

$$\beta k^{2\alpha} + 1 - (k-2)\alpha/2 > 0.$$

But since $0 < \alpha < 1/2$ this must fail for sufficiently large k. □

Proposition 16. *If $\alpha > 1/2$ then either $d_c < \infty$ or (10) determines β_c.*

Proof. For $d \geq 3$, (6) is equivalent to (8), i.e. $c_d \leq \frac{\beta - d^{-2\alpha}(d-1)}{d-2}$. If $\alpha > 1/2$ then the right hand side is positive for sufficiently large d and thus 'weaker' than condition (10). □

For $\alpha > 1/2$ it is possible that $d_c < \infty$ or $d_c = \infty$. See Figure 6 for the value of d_c as a function of α and γ.

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